Implementation and performance analysis of a model-based controller on a batch pulp digester

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Implementation and performance analysis of a model-based controller on a batch pulp digester

by

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A dissertation submitted in partial fulfillment
of the requirements for the degree

Master of Engineering (Control Engineering)

in the

Department of Chemical Engineering
Faculty of Engineering, the Built Environment and Information Technology

University of Pretoria
Pretoria

December 2003

Synopsis

The control of batch pulp digesters is hampered by insufficient measurements as well as nonlinearity and weak correlation between consecutive cooks. This makes a model-based approach to control attractive. Due to the age of the industry, many legacy controllers are in place on digesters around the world.

The theoretical variance obtained by Monte Carlo modelling of a new controller is used as a benchmark for performance comparison between an old control system (S-factor) and a new model based controller developed by the University of Pretoria (the UP controller). This study covers the development of the controller, Monte Carlo modelling of the old and new controllers and *in-situ* testing of the UP controller on an operating digester.

During Monte Carlo simulation, the UP controller outperformed the legacy controller, obtaining a theoretical overall variance of 3,07 (which will be used as the baseline for performance measurement) while also showing larger responses to tuning factors. The S-factor performed at 6,8 times the theoretical optimum variance during *in situ* testing, while the UP controller performed at 3,9 times the theoretical optimum (43% better than the S-factor controller). An average error 90% lower than that of the S-factor controller was obtained when using the UP controller.

Additional benefits of the new controller include easy inclusion of new measurements and clear relations between the tuning parameters used and the conditions in the digester.

KEYWORDS: batch control, performance analysis, Monte Carlo, model based control, pulping, sulphite process

Sinopsis

Die beheer van enkellading pulpverteerders word belemmer deur 'n tekort aan voldoende metings sowel as nie-lineariteite en swak korrelasie tussen opeenvolgende koke. Hierdie probleme kan oorkom word deur van modelgebaseerde beheer gebruik te maak.

Monte Carlo modellering is gebruik om 'n teoretiese skatting van die variansie van 'n nuwe beheerder te verkry. Hierdie resultate is gebruik om 'n bestaande beheerder wat gebruik word op 'n aanleg (die S-faktor beheerder) en 'n nuwe beheerder wat ontwikkel is by die Universiteit van Pretoria (die UP beheerder) te vergelyk. Die studie wat in hierdie verhandeling gedokumenteer is dek die ontwikkeling van 'n nuwe modelgebaseerde beheerder, Monte Carlo modellering van beide die ou en nuwe beheerders en *in situ* toetse van die UP beheerder op 'n verteerder in bedryf op die aanleg.

Die Monte Carlo simulasie toon 'n teoretiese standaard afwyking van 3,07 (wat as 'n basis gebruik word vir metings van beheerderdoeltreffendheid) en wys dat die nuwe beheerder die teiken vinniger nader as gevolg van aanpassing van die modelparameters. Tydens *in-situ* toetse loop die S-faktor beheerder teen 6,8 keer die teoretiese optimum variansie, terwyl die UP beheerder teen 3,9 keer die teoretiese waarde loop (43% beter). Gedurende die toetsfase was die gemiddelde fout behaal met die UP-beheerder 90% laer as dié behaal met die S-faktor beheerder.

Bo en behalwe die duidelike verbetering in variansie kan addisionele metings maklik ingesluit word in die beheeralgoritme van die nuwe beheerder en bestaan daar 'n duidelike korrelasie tussen die beheerderparameters en die toestande op die verteerder.

SLEUTELWOORDE: enkellading beheer, Monte Carlo, modelgebaseerde beheer, verpulping, sulfietproses

Acknowledgements

I would like to acknowledge the help and constant encouragement of my parents, the insightful tuition of professor Philip de Vaal and the unfailing willingness of Jonathan Centurion Harris and Richard Taylor to help during the ongoing debugging of the program. Eugene Botes was also instrumental during the data gathering phase. Thanks also to Sappi Saiccor for funding the project with the help of the THRIP initiative of the NRF.

I would further like to thank Donald E. Knuth for writing the TEX typesetting system and Leslie Lamport for creating LATEX.

> My mind rebels at stagnation.
> Give me problems, give me work,
> give me the most abstruse cryptogram,
> or the most intricate analysis,
> and I am in my own proper environment.
>
> Sherlock Holmes, The sign of four (Sir Arthur Conan Doyle)

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NOMENCLATURE

$[A]$	Concentration of A
R	Ideal gas constant
T	Temperature
A-D	Constants in the S-Factor target equation
B	Arrhenius normalisation factor
m	Pertaining to molecular weight
K	Represents multiple constants, defined by subscript
k	Constant parameter placeholder (used with subscript)
M	Average molecular weight
SF	S-Factor

Subscripts

bot	Bottom
HC	Hemicellulose
L	Lignin
m	Measured
n	Number of elements
top	Top

C Cellulose

C Controller (Used with G)

C Controller

Greek

α Level of confidence in normality tests

β_1 Skew estimator

β_2 Kurtosis estimator

μ Viscosity

μ Viscosity

θ Vector of sampled points for statistical analysis

θ Vector of samples for statistical tests

Abbreviations

COV Coefficient of Variance

CV Controlled Variable

DP Degree of Polymerisation

GPL GNU General Public Licence

MRAC Model Reference Adaptive Control

MV Manipulated variable

SISO Single Input Single Output

SP Setpoint

SQL Structured Query Language

t Number of trails in Monte Carlo analysis

d Disturbance

G Laplace domain transfer function

CHAPTER 1

Introduction

1.1 Background

During the pulping of wood, the chain length of the cellulose in the wood is reduced. This chain length – expressed as a degree of polymerisation (DP) – is the most important controlled variable in pulping. The DP is commonly inferred from the viscosity of the pulp, as it is difficult to measure DP directly.

At the Sappi Saiccor Umkomaas pulp plant, pulping is done in a batch process in batch pulp digesters. Several factors make the control of the pulp DP uniquely difficult.

- There are relatively few online measurements of digester inputs.
- These measured variables are not directly representative of the inherent state of the digester.
- DP is measured only at the end of a batch, not during the batch.
- There is a large delay between the end of one batch and the time when the DP reached during that batch becomes known.
- The results from one cook are only loosely connected to the results of the next cook.

These problems preclude the use of a high sampling rate control strategy in this study, as the important variables are not measured continuously. Instead, the most important control action will take place at a lower sampling rate, corresponding to the sampling of the DP.

A model of the reactions (the UP model) that take place during the pulping process was developed as part of a project to develop an improved control strategy for controlling the DP (Kilian, 1999). In this dissertation the UP model is used to develop and implement

a model-based controller (the UP controller). The performance of this controller is also evaluated.

1.2 Problem statement

The problem is to develop and implement an improved controller on the Sappi Saiccor plant and evaluate its performance. A good performance measure should be devised to evaluate controller performance fairly. The controller should also be implemented on a running digester to ensure that it is functioning correctly. Special attention should be given to the aggravating factors mentioned earlier.

1.3 Method

In order to define a valid baseline for control, the UP model for the reactions in the digester is to be used to simulate the effects of input variability on the output (DP). The performance of the UP controller is to be measured against the current controller in place on the digester using this baseline.

1.3.1 Distribution modelling

The distributions of the input variables measured on the plant will be simulated using a Monte Carlo method. The outputs recorded during these runs will then be characterised to obtain an estimate of the distribution of the output due to the measured input variability. This will provide a best-case comparison between the controllers, as the modelling will neglect unmeasured disturbances.

1.3.2 Performance measure

The performance measure chosen will relate the performance of a specific batch controller to the performance of a simulated optimal controller. The results of a series of cooks will be analysed and compared with a base case evaluated during the simulation step. The performance measure will show how close to the expected maximum level of control the plant is running.

1.4 Deliverables

The deliverables from this project are

- Results of Monte Carlo simulation of the legacy and UP controllers

- Determination of a baseline variability for control using the Monte Carlo results
- Comparative study of performance of the UP model and S-Factor controllers against the theoretical baseline.

1.5 Structure

Chapter 2 gives an overview of relevant literature in the field of batch control, Monte Carlo methods and performance measures. Chapter 3 gives a general background of the company, the product (dissolving pulp) it produces and the process employed. The control problem is formalised in chapter 4, identifying controlled, manipulated and disturbance variables. In this chapter, the problem is also reduced to three time frames (subsystems where system inputs and outputs have the same sampling rates), and the time frame where the focus should be is isolated. The work that has already been done on the control problem is presented in chapter 5.

The UP controller design is presented formally in chapter 6. The Monte Carlo simulation whereby the UP controller is to be compared to the current controllers is explained in chapter 7. The programming analysis for implementation of the controller on the plant is done in chapter 8. Chapter 9 contains a discussion of the results obtained in the study, and chapter 10 draws conclusions based on the results of the study and recommends further courses of action.

CHAPTER 2

Theoretical background

This chapter explores existing developments in controller implementation. It covers literature dealing with the following subjects:

- Control hierarchy and time scales on which control take place.
- Classic, advanced, model based control and adaptive control structures.
- Batch implementations of these control structures and batch specific control concepts.
- Implementation of control structures on existing plants.
- Planning and programming to create software controllers.
- Documentation standards for all the design and implementation stages.
- Testing and performance analysis of controllers.

The study is structured to represent the decision process that led to the final choice of controller.

Due to the difficulties inherent in the process, advanced control and state estimation methods were only briefly considered. The low sampling rate as well as measurements which are not directly related to the state of the reactions inside the reactor were the main factors influencing this choice.

2.1 Decisions

In the course of this project, several avenues were considered for controlling the viscosity and for evaluating the control performance. The decisions are shown graphically in figure 2.1.

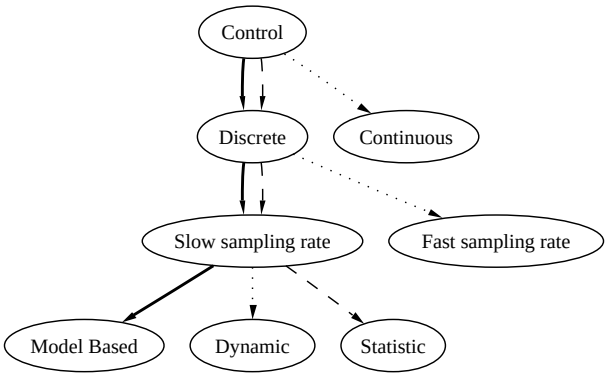

Figure 2.1: Decision tree for control. The solid line represents the control choices made, while dashed lines indicate performance measure choices.

The control problem indicates a clear decision line to the final controller choice based on the following aspects of the process and control problem:

- Low sampling rate of the controlled variable. The controlled variable is sampled once – after the control action has taken place.
- Lack of continuity in the process output. The process output during one cook is only loosely correlated to the cook before and after that cook.
- Nonlinear relationship between measured inputs and process outputs. The inputs and the outputs of the process are related by a system of nonlinear equations that are not analytically solvable.
- The continuously measured variables are not indicative of the state of the system. This makes state estimation difficult.

The lack of continuity and nonlinearity implies that a high level of process knowledge must be built into the controller. A model of the process will therefore be an attractive feature in a controller installed to control this process.

When choosing a measure of performance the same choices have to be made. The dashed line in figure 2.1 thus indicates a statistically based performance measure. In reality, the performance measure is based on the model of the process and then measured statistically in terms of variance (the second moment of distribution about the mean).

For problems of this kind it is important to understand that the lack of measurements and low sampling rate rule out many of the more advanced control strategies associated with nonlinear control problems. This chapter explores some basic control structures in addition to more complex techniques in order to highlight the features that can be extracted from the simple controllers to form an effective control strategy for this problem.

2.2 Time frame

Chemical processes are controlled on several time frames. The relationship of different levels of control that is often represented as a control hierarchy as shown in figure 2.2. The lowest part of this hierarchy (measuring devices and actuators) are usually sampled

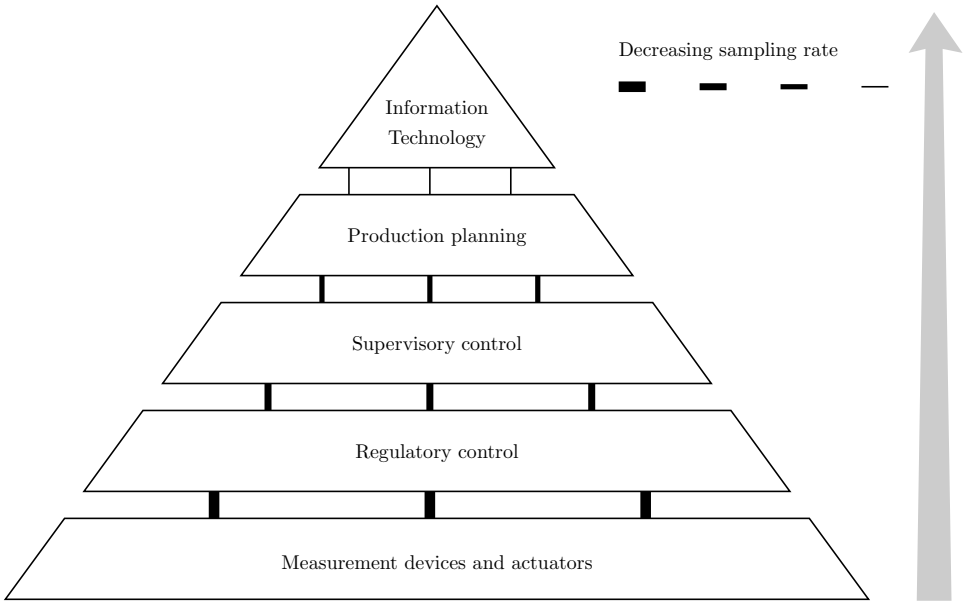

Figure 2.2: The control hierarchy (after Maciejowski (2002: 27))

very frequently. As one moves to more complex control structures and loops, the sampling rate goes down.

Different control strategies must be used for each level of this hierarchy. For instance, low-level control might require very fast response times when controlling fluid flow or critical temperatures. This rules out the use of slow optimising control algorithms which are often used in higher level control.

Throughout this dissertation, the thickness of connecting lines on block diagrams will correspond to the sampling frequency – a high sampling frequency will be represented by a thick line.

2.3 Classical control

Classical or traditional control is based on linear systems, analysed using frequency responses. Lurie & Enright (2000) use the definition "best frequency-domain design methods developed before 1960, and their extentions". Usually, the controllers stemming from classical control design incorporate feedback measures. Classical control is used in the continuous time scale. The distinction between classical control or base layer control and advanced control is difficult to define.

Due to the nature of the control problem presented in this dissertation, several concepts from classical control are useful in understanding the applicability (or lack thereof) of a control solution. In particular, it is important to understand the philosophy behind feedforward control, the shortcomings of frequency based control design techniques, and the problematic nature of infrequently sampled systems. The concepts are presented here to solidify these concepts before developing a solution.

2.3.1 Frequency response

One of the core aspects of classical control is frequency response analysis. Frequency responses can be used to describe: (Skogestad, 1996: 15)

1. A system's response to sinusoids of varying frequency,
2. the frequency content of a deterministic signal via a Fourier transform, and
3. the frequency distribution of a stochastic signal via the power spectral density function.

Most of the work done on frequency response analysis focuses on the first of the above interpretations (Skogestad, 1996). The first two points require either a continuous signal or a high sampling rate for discrete systems. The third point can be applied to stochastic systems, even with low sampling rates.

It is however important to remember that 'When process output variables are measured at a sampling interval that is considered large relative to the natural response time of the process, the natural dynamics of the process are less likely to be manifested in the observations...' (Ogunnaike & Ray, 1994: 1049). This applies to the third point, as the statistical characteristics of a process do not reveal the dynamics of the process.

2.3.2 System representation

As linear systems are often analysed using frequency responses, the Laplace transform domain is often preferred above the time domain to represent systems. Laplace *transfer functions* can then be defined as

$$G(s) = \frac{y(s)}{u(s)} \tag{2.1}$$

where $y(s)$ and $u(s)$ represent the input and output of the system respectively. In practise, the functions are shortened to G, y and u if there is no risk of ambiguity (Skogestad, 1996).

It is also useful to represent systems graphically in the form of a *block diagram*. In such a diagram, the relationship between inputs and outputs via transfer functions is shown graphically by arrows entering and exiting the system. Summing outputs of multiple

transfer functions is represented by a circle showing the applicable sign. The system shown in equation 2.2

$$y(s) = G_p(s)u(s) + G_d(s)d(s) \tag{2.2}$$

can then be represented as shown in figure 2.3

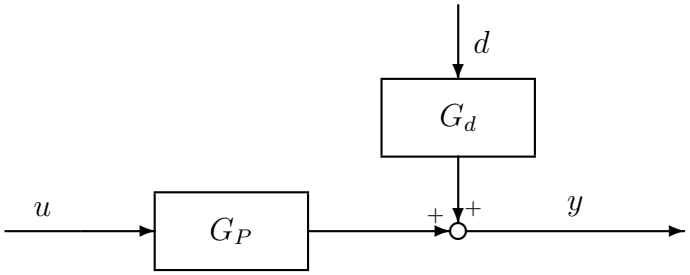

Figure 2.3: Block diagram representation of the system $y(s) = G_p(s)u(s) + G_d(s)d(s)$

2.3.3 Feedback

The general control structure for a feedback control loop is shown in figure 2.4. The basic principle of the controller is to modify the input to the controlled system (the action of the controller) based on the error measured from the output of the controlled system. This 'feedback' action is the defining characteristic of feedback control.

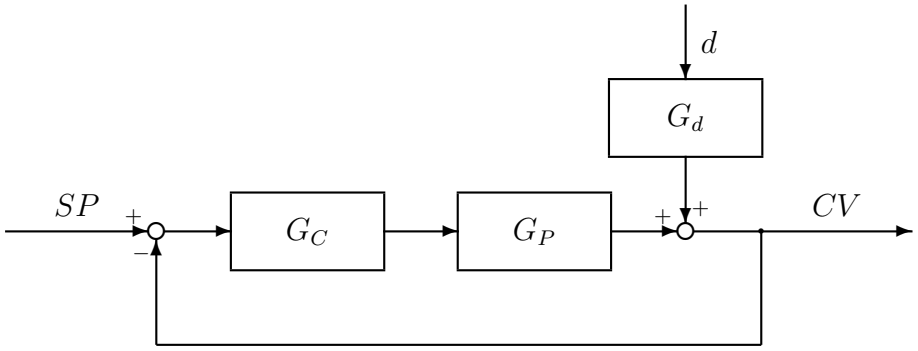

Figure 2.4: Feedback control structure (adapted from Marlin (2000: 17)). G_P, G_C and G_d are the controller, process and disturbance transfer functions respectively

The algorithms used in feedback control vary, but the most basic (and most pervasive) of the formulae used to calculate a response to the measured error is the PID (Proportional, Integral, Derivative) algorithm. In principle, the action of the controller is calculated by multiplying a constant factor with the error, the integral of the error and the derivative of the error (Luyben, 1990).

Feedback loops are generally capable of acceptable performance even when no knowledge of the system other than its response under control is available. The use of the controlled variable as a controller input via feedback enables controllers built on this

principle to perform in the face of changing system parameters. The tuning parameters may change, but the controller architecture can remain constant. (Marlin, 2000)

2.3.4 Feed Forward

One drawback to feedback control structures is that certain processes might only show a reaction to disturbances after a considerable time. When the controller then takes action to correct the error, the effect of this correction will also be measured late. If one has a model of the system and a measurement of the inputs, corrective action can be taken *before* the disturbance reaches the system. Applying this principle results in a control structure as shown in figure 2.5

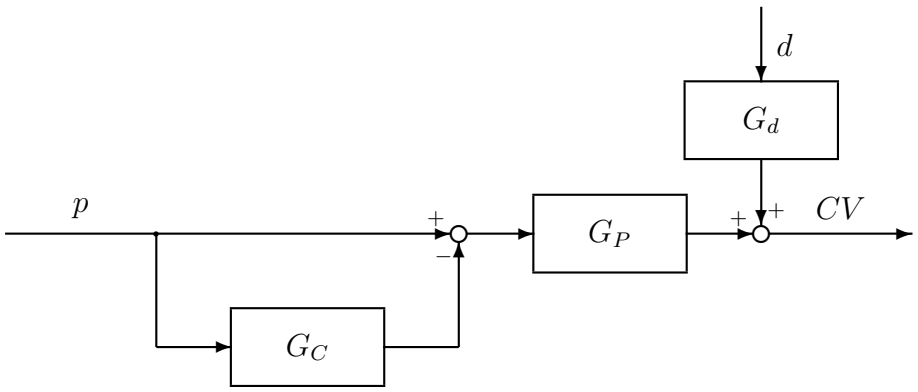

Figure 2.5: Feed forward control structure (adapted from Marlin (2000: 18))

Note that the disturbances (d) shown entering the system are not measured. The feedforward structure explained here does not compensate for these disturbances.

If the structure shown in the figure is approached with transfer functions in the Laplace domain, the ideal controller would cause the transfer function between the setpoints and the final outputs be equal to unity. For a SISO system, this gives $G_C = \frac{G_P - 1}{G_P}$. It is clear that the inverse of the plant would be required in order to apply this controller. This of course implies that the plant is invertable. In many cases, this it not true, leading to the use of a partial inverse (using only the part of the model for which an inverse can be calculated) for control calculations.

2.3.5 Combined structures

Hybrid systems containing both feedforward and feedback structures are often employed where the feedback controller compensates for mismatches between the feedforward controller and the model (Skogestad, 1996). This structure is shown in figure 2.6.

It can be seen that this controller structure uses a feedforward controller (G_{FF}) to react to disturbances before they enter the system, while the feedback controller (G_C) is

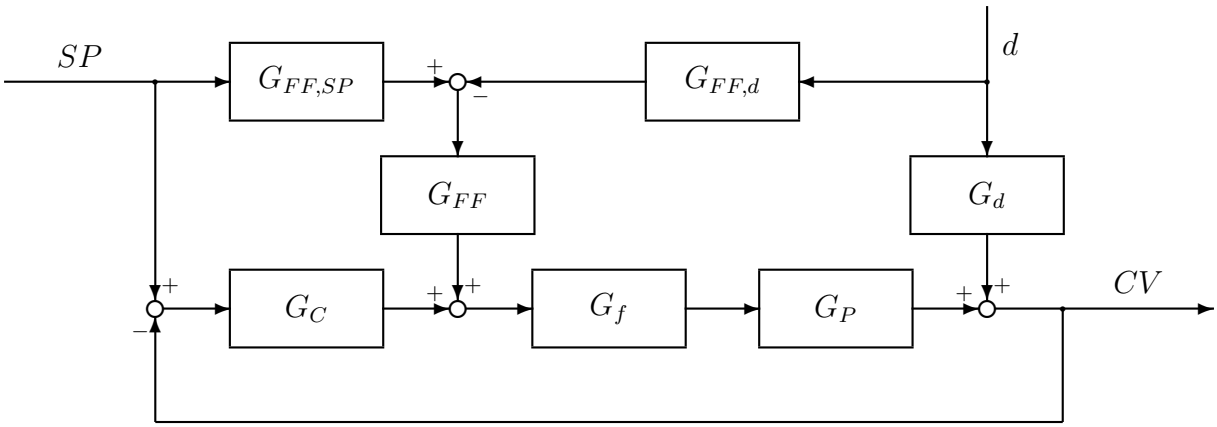

Figure 2.6: A unified control structure with feedback and feed forward action (Marlin, 2000: 20). G_f is a filter transfer function

used to correct for model-controller mismatch, in effect compensating for the uncertainty inherent in any model of a process.

2.4 Discrete control

Discrete controllers were developed in response to the advent of digital computers, which could not handle analog signals (Ogunnaike & Ray, 1994).

> The use of the computer for data acquisition introduces a new perception of the process: a quantized[*sic*] view, in which the system is no longer seen as giving out continuous information, continuously in time; process information now appears to be available only in discrete form, at discrete points in time.(Ogunnaike & Ray, 1994)

These signals have to be sampled to convert them from analog to digital signals. The digital signals have a fixed interval between them (the sampling interval). Many of the classic continuous controllers can be converted to discrete forms (Marlin, 2000), but there are discrete controllers which operate on a control *logic* instead of pure mathematical relationships.

According to Marlin, discrete controllers can be implemented on the continuous time scale as well as on higher level time scales. Discrete analysis does not require the strong relationship to frequency response that classical control analysis requires (Marlin, 2000), even though some frequency response related analysis can be done on discrete systems.

2.5 Model based control

Model based control is a generic term for all controllers that make explicit use of a model of the process to be controlled in order to derive both controller structure and parameters (Ogunnaike & Ray, 1994: 645). Feedforward control as explained in paragraph 2.3.4 can therefore be seen as a model based control technique, as it requires an explicit inverse of the process model.

Marlin (2000: 584) explains the use of a model in control processes as a natural extension of human control logic. His argument is that humans attempt to model the process they are controlling and react to the difference between the predicted response of the system and the true response.

When defined in this way, model based control is a very large field, and only a few of the most popular techniques are discussed here.

2.5.1 Predictive control structure

In 1982, Garcia & Morari introduced the Internal Model Control (IMC) structure, showing how this structure could represent many of the control structures that were popular at the time. In the same article, the authors extend the control structure to predictive control action. This scheme involves predicting the process' response to control action and basing control action on these predictions.

Figure 2.7 shows the generalised IMC structure using a predictive controller and offset compensators (G_{OC1} and G_{OC2}). This structure has been proposed by many sources, but

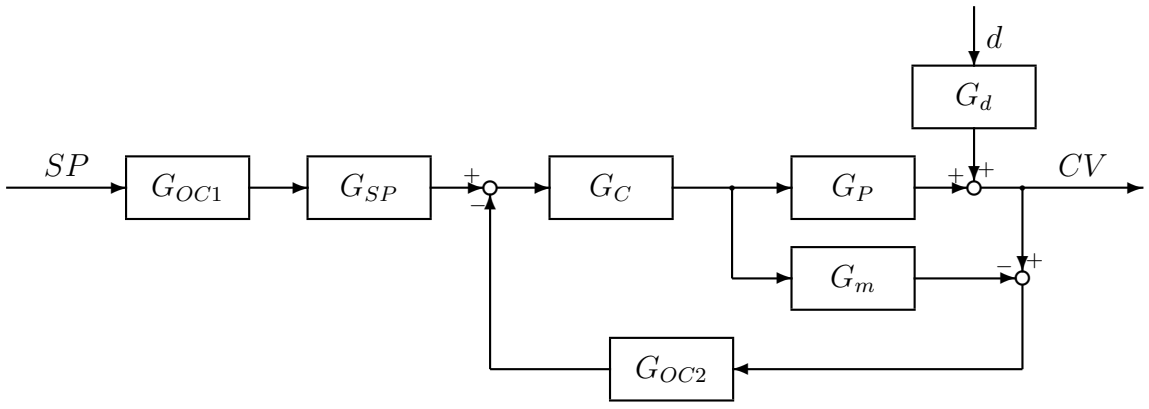

Figure 2.7: IMC structure with predictive controller and offset compensator (Garcia & Morari, 1982)

has become known as the general predictive control structure. It can be seen that the model G_m is used to approximate the response of the system to the control actions from the controller. The difference between the modelled response and the true response of the system G_P is then fed back into the system to accommodate modelling error and the effect of the unmeasured disturbances d.

2.6 Adaptive control

The control techniques discussed above are all based on assumptions of static models, or at least that the controllers will be able to maintain control even though the model of the process and the process itself are not in accordance. However, when the controlled process changes with time, the control performance of these controllers degrades. One method of improving controller performance in the face of changing conditions is to adapt the model parameters based on the response of the model under controlled conditions or some other criterion (Hang et al., 1986).

To summarise: 'In the adaptive control scheme, the controller parameters are adjusted (in an automatic fashion) to keep up with the changes in the process characteristics. We know intuitively that, if properly designed, this scheme will be a significant improvement over the classical scheme.' (Ogunnaike & Ray, 1994: 628)

Several adaptive control structures exist, three of which are discussed here:

2.6.1 Scheduled adaptive control

If the process to be controlled is well understood, preprogrammed areas of operation can be used in an adaptive structure. This type of adaptive control is also sometimes known as gain scheduling (Ogunnaike & Ray, 1994: 628). A typical example of gain scheduling can be found in level controllers which are set up so that they have low gain near setpoint and high gain near upper and lower limits.

2.6.2 Model reference adaptive control

A different adaptive control structure is shown in figure 2.8. In this structure, a reference

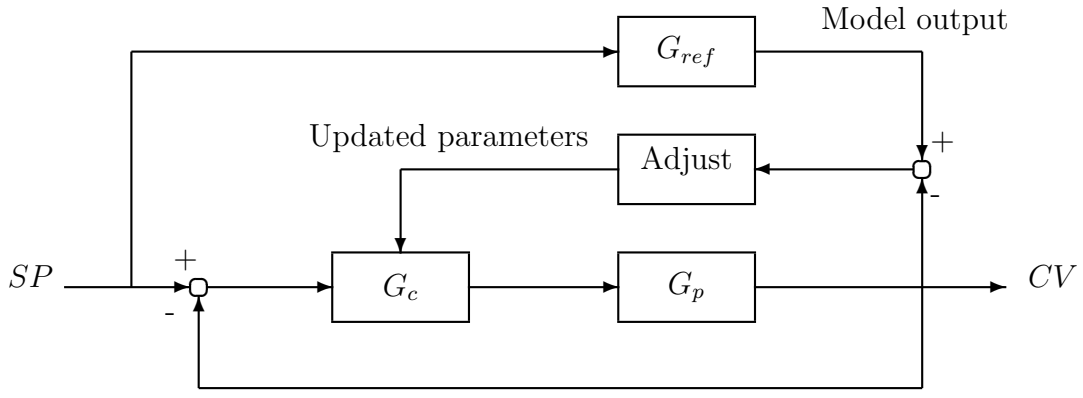

Figure 2.8: Model reference adaptive control (MRAC) structure (Narendra & Valavani, 1979)

model (G_{ref}) is used to estimate the modelling error. The controller parameters are then adjusted in response to this error.

2.6.3 Self-tuning adaptive control

Figure 2.9 shows the self-tuning adaptive control structure. In this structure a reference model is not explicitly involved (Ogunnaike & Ray, 1994). Instead, an estimate of the

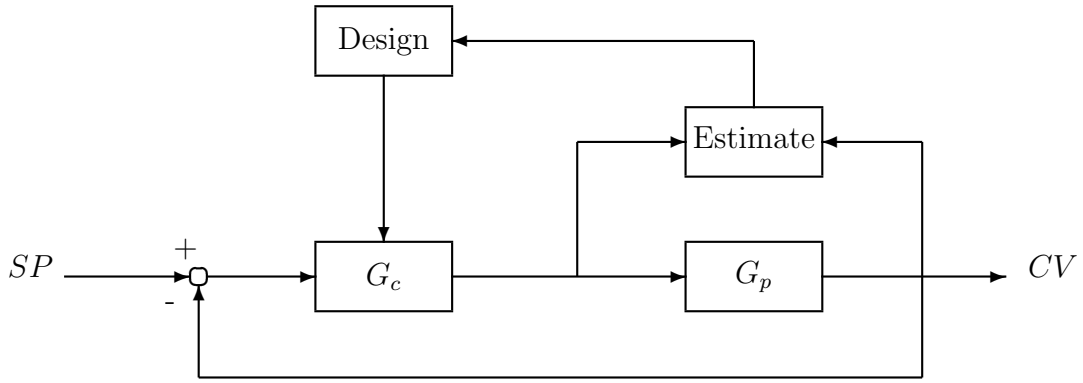

Figure 2.9: Self tuning adaptive control structure (Ogunnaike & Ray, 1994: 630)

process is built by measuring the inputs and outputs of the prosess. This estimate of the process is then used to design the controller.

2.6.4 Iterative learning

During a batch, startup or shutdown procedure, a process may move into regions where the original controller models are not valid any more. If the desired trajectory of the process is known and constant, adjustments can be made to the controller output to improve control(Xu et al., 2001). For a vector of adjustments a at regular intervals during a procedure, the controller output is then calculated as $m + a$ where m is the controller output.

Figure 2.10 shows an example of a desired and actual trajectory for such a process. If there is an error vector (ϵ) at the adjustment points, this can be used to update the adjustments at each run. A commonly used update algorithm uses an adjustment constant Δ, where the new updates are calculated using equation 2.3 (Amann et al., 1996).

$$a_{i+1} = a_i + \Delta \cdot \epsilon_i \tag{2.3}$$

In this way, the desired trajectory can be attained by adjusting the inputs as shown in equation 2.3 repeatedly. This strategy may be combined with control methods such as model predictive control (Lee et al., 1999) and traditional feedback or feedforward control (Amann et al., 1996). It should be noted that these adjustments are only useful when the controlled variable can be measured at the points at which adjustments are to be made.

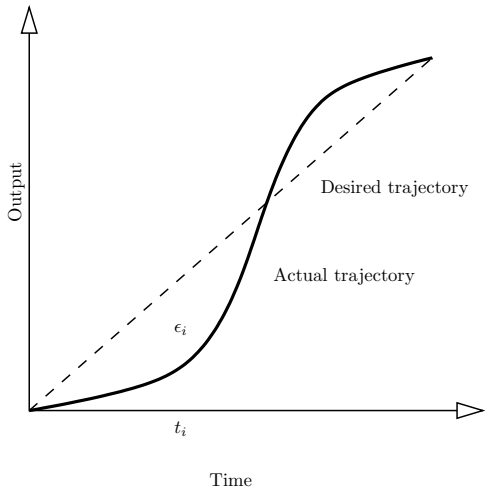

Figure 2.10: Iterative learning control action

2.6.5 Intelligent control

Intelligence has been a buzzword in the control industry since the advent of 'thinking algorithms' such as neural networks, expert systems and fuzzy logic. This word is however grossly overused (Gupta & Sinha, 1996). Several adaptive structures make use of one of these thinking algorithms to update the model parameters or to supply corrections to simpler control algorithms.

2.7 State estimation

When modelling an unknown process it is often desirable to obtain an estimate of the states of the system based on noisy measurements or on measurements which are only functions of the true states (Dochain, 2003). Popular methods to address this problem include the Kalman observer and extended Kalman observer (EKO), also known and implemented as a Kalman filter and Luenberger observers.

2.7.1 Kalman observers

In 1960 Kalman et al. (1960) proposed an iterative solution to the Wiener problem (of finding the optimal fit of a predicted true signal to a noisy signal) which leads itself very well to state estimation based on noisy measurements. The method described in this seminal article has been implemented widely, with implementations of the algorithm often known as Kalman filters.

The method is based upon the assumption that the true dynamics of the system to be observed can be modelled by a discrete linear function and that the measurements are perturbed by an unknown amount of white noise. In the procedure, the probabilities of error based on the measurement and the model predictions are minimised (which also

solves the Wiener problem).

Implementations where the model is re-linearised about the current operating point are known as extended Kalman observers and are more robust when used to observe nonlinear processes.

2.7.2 Luenberger observers

Luenberger (1964) introduced a state observer which addresses the problem of obtaining estimates of true states by measuring another set of variables.

The method is based upon a linear model of the process, with dynamic parameters closely resembling those of the true process. The measured outputs from the true process are compared to the outputs estimated by the model, and parameters relating the process states and outputs are adjusted to minimise the model error. This approach works well in the absence of measurement noise (Tarantino et al., 1999).

2.7.3 Application to per-batch control

There are several applications where the use of state estimators is beneficial in batch control purposes. The most important aspect of state estimators is however that they require measurements which are closely related to the states they are to estimate. These measurements are either assumed to be equal to the states with the addition of noise, or functionally related to the states by an unknown function. For the control problem that this dissertation is concerned with, the use of state estimators is precluded by the lack of measurements which satisfy these criteria.

2.8 Statistical control

When the variables being controlled are sampled infrequently, when the measurements contain a large amount of uncertainty and when control adjustments are costly, the goals of process control are subtly shifted toward a more stochastic view. Ogunnaike & Ray (1994: 1033) state that effective process control within such a framework can be broken down into two parts:

1. An objective analysis of the observed deviation of the process variable from its desired value.

2. A rational decision regarding what to do to minimize[*sic*] such deviation.

The field of statistical control was approached from two different fields. One was the field of quality control, the other traditional process control using stochastic models (Juba & Hamer, 1986).

2.8.1 Quality control

When control manipulations are costly, it is important to assess whether a current deviation from setpoint is due to normal noise or whether action should be taken. The quality control school of thought implemented a series of charts from which certain 'in control' checks could be implemented.

- Shewart charts plot an error divided by the expected standard deviation. In this way, a value of the controlled variable which deviates by more than a certain multiple of the standard deviation can easily be seen. Lim (2002), referencing Shewart (1931), obseverves that these charts are designed to detect large but transient shifts in the process mean.
- CUSUM (cumulative sum) charts, can easily highlight small persistent shifts in process mean but are more difficult to apply. (Alberto Luceño, 2002)

2.8.2 Standard process control

When control manipulations are relatively cheap, the advantages of not reacting to spurious control situations become less. In situations like these, and when the sampling interval is large relative to the natural response time, standard process control is more appropriate (Ogunnaike & Ray, 1994: 1050).

2.9 Batch control applications

Rippin (1989) uses the term 'ill-definedness' to describe the change, variability and uncertainty that batch processes involve. These factors necessitate the use of advanced control structures. Several advanced control structures have been implemented on batch plants.

Berber (1995) gives an overview of the control techniques commonly adapted for service in batch reactor control. He cites several of the control structures already discussed in this chapter, but focuses on applications which are more relevant to the continuous time frame.

The theory of optimal control can be used to generate recipes for batch processes and Juba & Hamer (1986) show that, when controlling the composition inside a batch chemical reactor, the open loop temperature trajectory required could be expressed as an optimal control problem.

Also, using a feedforward-feedback structure including an iteratively determined inverse, Balakrishnan & Edgar (2000) implemented a model-based controller with PID feedback to control the temperature profile of a silicon wafer during rapid thermal processing. This structure is most promising as a control structure for the batch control problem under investigation.

2.10 Monte Carlo Simulation

Monte Carlo simulation offers an alternative to analytical mathematics for understanding a statistic's[1] sampling distribution and evaluating its behaviour in random samples. Monte Carlo simulation does this empirically using random samples from known populations of simulated data to track a statistic's behaviour. (Mooney, 1997)

2.10.1 The Monte Carlo Principle

The principle behind Monte Carlo simulation is that the behaviour of a statistic in random samples can be assessed by the empirical process of actually drawing a number of random samples and observing this behaviour. The strategy for doing this is to create an artificial 'world' or *pseudo-population*, which resembles the real world in all relevant respects.

In order to simulate the real world, virtual processes must be generated that will respond on the inputs provided just as a real process would. This virtual process can then be used to conduct multiple trials of the statistical procedure of interest to investigate the behaviour of a statistic across samples.

The process can be visualised as shown in figure 2.11, with input variability propagating through the process to produce measurable output variability.

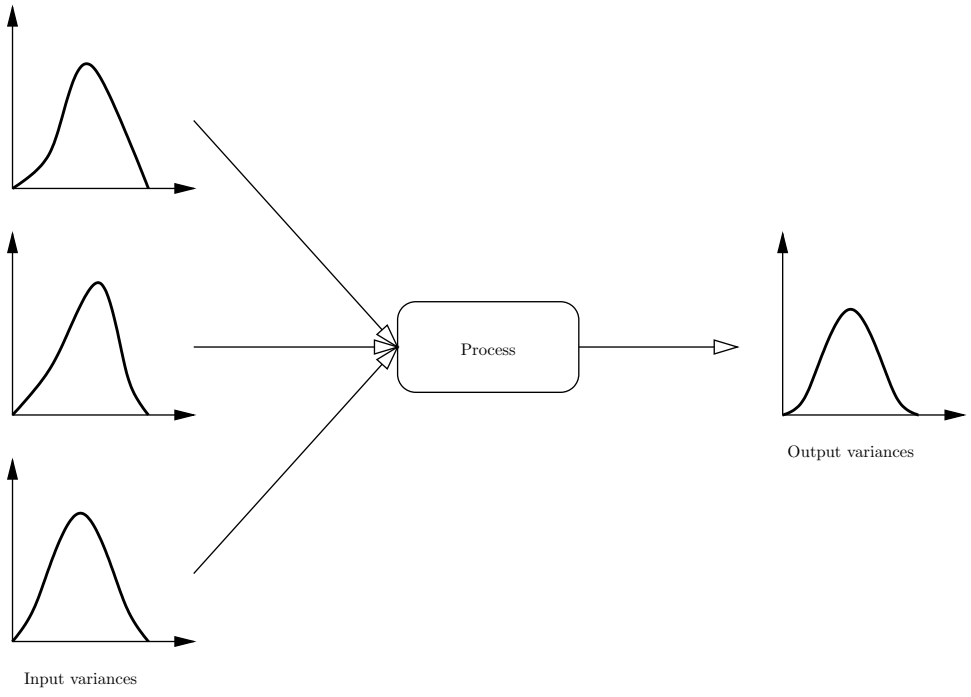

Figure 2.11: Variability propagation explained: Input variability propagates through the system to cause output variability

[1] A statistic is any quantity under scrutiny in a statistical study

2.10.2 Procedure

Mooney (1997) describes the Monte Carlo procedure as follows:

1. Specify the pseudo-population in symbolic terms in such a way that it can be used to generate samples. This usually means developing a computer algorithm to generate data in a specified manner.

2. Sample from the pseudo-population (a *pseudo-sample*) in ways reflective of the statistical situation of interest, for example with the sample sampling strategy, sample size and so forth

3. Calculate the statistic in question for the pseudo-sample and store it in a vector θ.

4. Repeat steps 2 and 3 t times where t is the number of *trials*

5. Construct a relative frequency distribution of the resulting values for all the trials, which is the Monte Carlo estimate of the sampling distribution under the conditions specified by the pseudo-population and the sampling process.

2.10.3 Confirmation of results

In order to confirm that the distributions fitted to the data obtained from a Monte Carlo simulation are indeed normally distributed, several tests have been proposed. A brief summary of these tests is given here.

Skewness and kurtosis

Skewness is a measure of how far the median value (peak of the distribution graph) is away from the mean of the data. Kurtosis is a measure of the 'slimness' of the data, in other words how closely the distribution is spread around the mean value.

The skewness estimator is given by Mooney (1997) as:

$$\sqrt{\beta_1} = \frac{\sum_{i=1}^{t} \left(\theta_i - \bar{\theta}\right)^3 / t}{\left[\sum_{i=1}^{t} \left(\theta_i - \bar{\theta}\right)^2 / t\right]^{\frac{3}{2}}} \tag{2.4}$$

This is usually combined with a kurtosis estimator

$$\beta_2 = \frac{\sum_{i=1}^{t} \left(\theta_i - \bar{\theta}\right)^4 / t}{\left[\sum_{i=1}^{t} \left(\theta_i - \bar{\theta}\right)^3 / t\right]^2} \tag{2.5}$$

. In both these equations, $\bar{\theta}$ is the arithmetic mean of the samples (ie, the sum of the elements divided by t). Values of 0 and 3 for the skewness and kurtosis respectively are expected for a normal distribution (Kleijnen, 1975).

Shapiro-Wilk test for normality

The Shapiro-Wilk test (Shapiro & Wilk, 1965), calculates a W statistic that tests whether a random sample, $\theta_1, \theta_2, \ldots, \theta_n$ comes from (specifically) a normal distribution. Small values of W are evidence of departure from normality. This test has done very well in comparison studies with other goodness of fit tests.

The W statistic is calculated as follows:

$$W = \frac{\left(\sum_{i=1}^{n} a_i \times \theta_i\right)^2}{\sum_{i=1}^{n} \left(\theta_i - \bar{\theta}\right)^2} \tag{2.6}$$

where the θ_i are the ordered sample values (θ_1 is the smallest) and the a_i are constants generated from the means, variances and covariances of the order statistics of a sample of size n from a normal distribution.

Kolmogorov-Smirnov test

Further checking of normality can be done by using the Kolmogorov-Smirnov test (Chakravarti et al., 1967: 392–394) to compare the distribution to a normal distribution with the same mean and standard deviation. This is not a specific test of normality, but rather a general goodness-of-fit test for any probability distribution.

The cumulative probability distribution curves for both distributions are plotted, and the maximum distance between them determined. This distance (the Kolmogorov-Smirnov distance or the KS statistic) is then compared to tables for the number of samples in the test distribution to determine the goodness of fit. The critical distance is also affected by the level of confidence, α. It is customary to set $\alpha = 0{,}05$, corresponding to a 5% chance of mistakenly discarding the assumption that the test distribution is indeed normally distributed.

For samples larger than 20, the critical distance is found by calculating an asymptotic solution to an n^{th} order polynomial. This task is usually handled by computer software.

The Kolmogorov-Smirnov test was favoured for confirming normality of the test results as it lends itself well to graphical interpretation, enabling the tester to interpret the normality results more meaningfully than a simple number.

2.11 Control system implementation

Implementing a new controller on an existing plant with a control system in place has many pitfalls. It is imperative that the correct procedure is followed as the control problem is approached.

2.11.1 Analysis

Even with an existing controller in place, it is important to start at the beginning and do a proper control analysis. Gupta & Sinha (1996) state:

> ad hoc implementations of ... control systems must be avoided because
>
> 1. it is bad engineering practise,
> 2. most likely such implementations will not be reliable, and
> 3. ultimately they will not be trusted.

Control system analysis proceeds in a number of well-defined steps as shown below (Stephanopoulos, 1984):

1. Classify the variables. Identify input and output variables.
2. Define control objectives.
3. Select measurements.

2.11.2 Implementation

When the control problem has been properly analysed, additional steps are required before the implementation of the controller. These steps are (Skogestad, 1996):

1. Select performance criteria for adequate control
2. Select a control strategy
3. Evaluate control strategy theoretically

2.12 Programming

Many problems encountered by the control engineer involve the creation of computer software. This may be to model a control problem, to evaluate the performance of controllers or to process data acquired from a process. In any event, the program must be written in a sound way to ensure that both the originator of the program and other users who will use the program may do so easily and repeatably, with the least reproduction of effort (Kim & Carlson, 2001).

2.12.1 Program design

The broad goal of program design is to convert a set of requirements from specification to computer code.

Two main schools of thought exist in the design of programs. The top-down approach sees the program in terms of large goals first and then refines these goals into smaller sub-tasks that are eventually small enough to correspond with computer language commands. The bottom-up school approaches a problem by constructing small procedures that will be required first, then integrating all of these into a whole. Both of these approaches are often used in the same project.

2.12.2 Documentation

When creating a program or developing any design for industry, documentation is crucial to ensure that the hand-over of information pertaining to a project can be done efficiently. The following standards specifically related to programming can be applied:

- Code documentation should be legible and ample Deitel & Deitel (2001).
- Documentation of equations and algorithms used should exist separate from the program code, and should use the same nomenclature as used in the program, or have a simple table defining the corresponding program and documentation variables (Chapman & Bates, 2000).
- The program should be as simple as possible to ensure that engineers who use the program do not need above normal computer programming skills to operate and change the program.

2.13 Controller performance assessment

It is crucial to assess the performance of controllers. This assessment should preferably be made during the design stage as well as after implementation. In order to obtain a measure of this performance, many methods have been proposed.

2.13.1 Control objectives

Controllers are implemented with various design objectives, including setpoint tracking, disturbance rejection, constraint handling and surge attenuation (Harris et al., 1999). Controller performance measures will clearly have to be related to these design objectives.

2.13.2 Continuous performance measures

Skogestad (1996) (as well as several others) notes that there are several time-domain performance measures. These include rise time, settling time, overshoot and decay ratio. All these methods rely on a continually changing controlled variable which is continuous in the time domain. Furthermore, these methods expect an oscillation in the response of the system to control. The application of these measures to batch controllers is not reliable due to the low sampling rate and poor continuity of these processes.

Several time-integral performance measures are available in Stephanopoulos (1984), Luyben (1990) and Skogestad (1996). These use the integral of the error of the control response to supply an objective function for controller optimisation. The errors discussed are the Integral of the Square of the Error (ISE), the Integral of the Absolute value of the Error (IAE) and the Integral of the time-weighted Absolute Error (ITAE). These are all in the form $E = \int_0^\infty f(t)\mathrm{d}t$, where the function $f(t)$ is often also a function of $\epsilon(t) = y_{SP}(t) - y(t)$. These performance measures are more applicable to batch control, but still have the disadvantage that these functions assume some continuity of the controlled variable.

2.13.3 Statistical performance measures

In the field of statistical control, assessment of the performance of the controller is an integral part of the control action (Ogunnaike & Ray, 1994: 1036). Paragraph 2.8 dealt with the methods employed to determine the performance of statistical controllers.

2.13.4 Minimum variance

Harris et al. (1996) essentially propose that the plant be considered as a stochastic process and that, for known distributions of the input variables and measurements of the corresponding outputs, a minimum variance controller can be synthesised by using a least-squares fitting approach of a prototypical model.

Once the minimum variance controller has been synthesised, the Harris Performance Index can be expressed as shown in equation 2.7

$$HPI = 1 - \frac{\theta}{\theta_{MV}} \tag{2.7}$$

where θ is the performance of the control system under scrutiny expressed as a fraction between one and zero and θ_{MV} is the performance of the minimum variance controller. A performance index close to zero is nearer to ideal control performance.

Patwardhan & Shah (2002), commenting on Harris et al. (1996) explain the benefits of the Harris performance index as well as possible causes of variability:

> 'An important property of the Harris performance index is its invariance to the magnitude of the disturbances. A poor performance index can be the outcome of one or more of the following:
>
> 1. limitations on achievable performance arising due to a combination of process and controller design
> 2. changes in plant dynamics
> 3. varying disturbances
> 4. sensor faults and
> 5. process nonlinearity.'

A procedure for synthesising the minimum variance controller from plant data collected during normal operation is explained in Venkatesan (2002), but requires that the system to be analysed be discretely coincident and continuous, meaning that the system must be sampled at the same interval as the controller and that signals must be continuous on this interval. This rules out any process where the outputs are not continuous for the procedure.

There are also problems with the standard minimum variance controller, highlighted by Grimble (2002): 'The main difficulty with this approach is that the minimum variance control law often gives high gain, wide bandwidth and unrealistically large control signal variations.'

The requirements of a coincident and continuous system, combined with the large control signal variations which would not be absorbed by a batch system with no continuous movement disqualifies the minimum variance controller as a valid control baseline.

CHAPTER 3

Background

In this chapter, general background is given about Sappi Saiccor and the plant on which the controller is to be implemented. The process and related measurements are described in enough detail that the reader can understand what the controller must be able to do.

3.1 Company details

Sappi Saiccor is currently the world's single largest and lowest cost producer of dissolving pulp and exports almost 100% of its product, mainly to China, India, Japan, the United Kingdom, North America and Europe. The company produces approximately 600 thousand tons of dissolving pulp per year (SAPPI web site, 2002), which represents a 11% share of the 5,5 million ton world market (Durbak, 1993).

3.2 Pulping process

The Sappi Saiccor Umkomaas plant uses the acid sulpite process of chemical pulping to produce dissolving pulp. This process works well for the production of pulp from the typical wood species used at the plant (Kilian, 1999).

3.3 Materials

3.3.1 Wood

Sappi Saiccor uses approximately 1,8 million tons of timber to produce the indicated production of dissolving pulp per annum. Nine different wood species are used at the

mill, with the majority of the wood being eucalyptus and wattle. The normal distribution of the wood fed to the digesters are approximately 85% eucalyptus (mostly *Eucalyptus Grandis* and *Eucalyptus Saligna*) and 15% wattle (*Acacia Molissima*) (Kilian, 1999).

3.3.2 Cooking Liquor

The liquor consists of a calcium or a magnesium base and approximately 6 to 7% dissolved SO_2 gas and 1,2% combined SO_2. The combined SO_2 corresponds to the base content of the cooking liquor and is present in the form of disulphide.

3.3.3 Dissolving pulp

Dissolving pulp produced on the plant is used in the manufacture of a variety of cellulose based products and by-products for the textile, chemical and plastics industries. In the textile industry the dissolving pulp is used in the manufacture of viscose fibre used for woven and non-woven fabrics. Other products produced from pulp are shown in table 3.1.

Table 3.1: Products produced from dissolving pulps (Durbak, 1993)

Product	Use
Medical wipes and swabs	Medicine
Tyre cord	Rubber tyres
Cellophane	Wrapping material
Yarns	Textiles
Plastics	Knobs, handles, etc.
Cellulose film	Photography
Lacquer	Ornamental
Membranes	Dialysis, water purification

During the manufacture of these products the pulp is dissolved in a number of steps which involve the addition of alkali and carbon bisulphite. When this solution is passed through small diameter nozzles while being neutralised, it forms the fibres that are used to manufacture these various products. This dissolving/precipitation process leads to the name of dissolving pulps. The purity of these pulps is usually more than 92% α-Cellulose.

3.4 Equipment

Newly acquired wood is stored in a wood yard to await further processing. It is chipped and stored on a chip pile, from where it is conveyed to chip silos. The silos supply wood to wood loaders that load the wood chips into the digesters. Although there are 23 digesters,

there are only two sets of wood loading equipment. The pulp exiting from the digesters is discharged into two wash pits where it is prepared for bleaching.

The digesters are grouped by the process they use. Eight newer digesters use a magnesium based process and are referred to as the 'magnesium side', while the remaining fifteen digesters called the 'calcium side' uses a calcium based process. The loading and discharging equipment is shared by all the digesters on a side.

The magnesium side is used to cook all the wattle and some eucalyptus wood. The calcium side is used to cook the remaining eucalyptus wood. The pulp from both woods is blended to increase product uniformity.

Each digester is 16,5 m high and has a volume of 285 m^3. When full, each digester holds about 100 tons of wood chips and 200 m^3 of cooking liquor. A circulation line extracts liquor from the bottom of the digester, where chips are retained by a grid. An external heat exchanger heats this liquor before it is returned to the top of the digester. This external heat exchanger uses superheated steam at a temperature of 165℃ and a pressure of 550 kPa to heat the circulating cooking liquor. A schematic diagram of a batch pulp digester is shown in figure 3.1.

Two temperature sensors are installed on the digester. On the diagram in figure 3.1, these temperatures are shown as $T_{m,\ top}$ and $T_{m,\ bot}$. The temperature of the liquor entering the heat exchanger from the bottom of the digester is measured in the first section of the circulation line, while the temperature of the liquor at the top of the digester is taken as the temperature of the liquor at the end of the circulation line.

A flow sensor installed on the circulation line measures the flowrate of the liquor being circulated through the heat exchanger.

Each digester is fitted with a Svensson steam packer, which uses steam to pack the chips tightly into the digester. This ensures that the chips are uniformly packed, that any trapped air is removed and that the chips are charged with an initial amount of water.

Each of the digesters is also fitted with a gamma ray level sensor to measure the level of the material inside.

3.5 Measurements

3.5.1 Degree of polymerisation

One of the important pulp quality measures is the chain length of the cellulose in the pulp. Kilian (1999) gives a range of methods that are used to determine this chain length, including methods based on osmotic potential, light scattering and viscosity. In the industry, this is usually expressed as a Degree of Polymerisation (DP)(Watson, 1992).

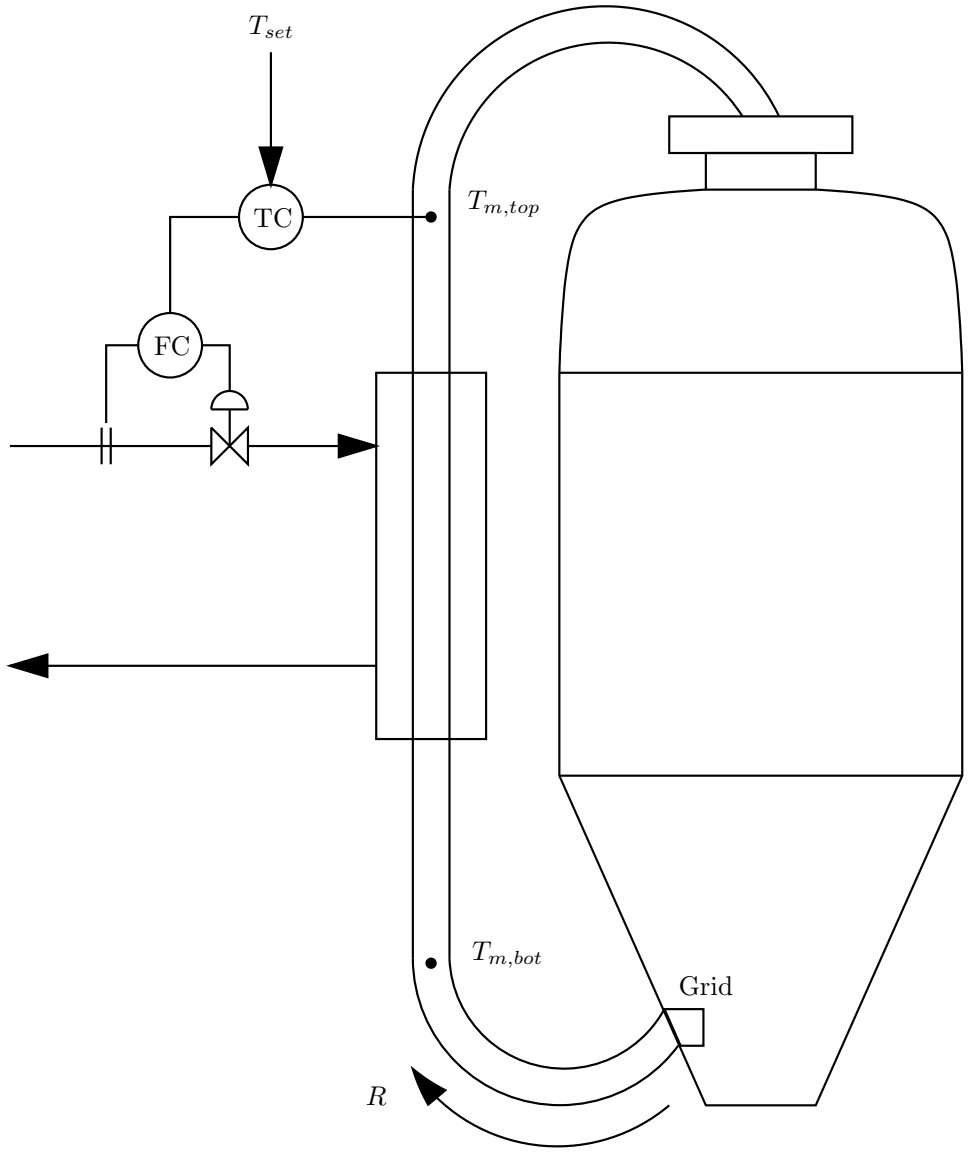

Figure 3.1: Schematic of a batch digester

3.5.2 Viscosity

According to Rydholm (1965), the intrinsic viscosity η, of a solution can be determined by measuring its specific viscosity at several low concentrations and extrapolating to zero concentration. The average molecular weight is then calculated by using the equation

$$\overline{M} = K_m \cdot M^a \tag{3.1}$$

and values for the constants K_m and a obtainable in literature.

The solvents used in measuring cellulose DP are powerful swelling agents that disrupt the crystal lattice of the cellulose, forming a gel-type solution with a viscosity which can be related to the average DP value of the cellulose molecules (Watson, 1992).

3.5.3 Cuprammonium test

According to Watson (1992), the solvent used on the Sappi Saiccor plant is cuprammonium. A direct correlation with DP has been found to be given by

$$DP = 285{,}4\mu^{0{,}345} \tag{3.2}$$

which is valid for $20\,\text{cP} < \mu < 150\,\text{cP}$.

3.6 Process overview

The fact that there is shared service equipment on the plant necessitates scheduling of operations to avoid more than one digester at a time being in one of the following phases:

1. Wood loading
2. Liquor loading
3. Pressurisation
4. Side relief
5. High pressure gas release
6. Low pressure gas release
7. Pulp discharge

The time for each phase is fixed to facilitate scheduling. The following sections detail the procedure for the phases enumerated above.

3.6.1 Wood loading

Chips are pneumatically conveyed to the top of the digester. A cyclone separates trapped air from the chips, and extraction fans at the bottom of the digester remove air during loading. The chips are packed into the digester by the Svensson steam packer connected to the bottom of a cyclone which removes wood dust from the chips coming from the silo.

Loading is stopped when the chip level is 2 m from the top of the digester. This phase is roughly 20 minutes long.

3.6.2 Liquor loading

On completion of the loading of the wood, the cooking liquor is loaded. The loading of the liquor continues until the liquor level rises above 14,5 m in the calcium digesters and 13,5 m in the magnesium digesters. Circulation of the liquor through the heat exchanger starts at the same time as the liquor loading. Liquor loading takes about 30 minutes to complete.

3.6.3 Pressurisation

When liquor loading is complete, the digester is pressurised to a pressure of 900 kPa_g. During this phase, steam flow to the heat exchanger is initialised, increasing the temperature of the digester contents. This increase in temperature also leads to an increase in pressure.

Pressurisation only supplies initial pressure. After pressurisation the digester pressure drops sharply before continuing to rise due to temperature increase.

The median pressure profile measured in the digester over time for 300 cooks during 2003 is shown in figure 3.2. The shaded area represents the area between the 5^{th} and 95^{th} percentile. It can be seen that the pressure varies significantly with regards to the time of certain features and the rate of pressure increase. This is because the pressure is not directly controlled, but is rather a function of the pressurisation stage and the temperature increases that are prescribed by the temperature profile. The only feature of the pressure curve that is guaranteed to be repeatable is the maximum pressure, as this is limited to 8,2 barg (P_{max}) by a pressure relief valve.

The variability of the pressure profile in early stages of the cook is not cause for concern, as reactions take place mainly at temperatures above 130℃. In the following section, it will become clear that this occurs only in the later stages of a cook when the pressure is constant.

Figure 3.3 shows an idealised version of this pressure profile, highlighting significant features.

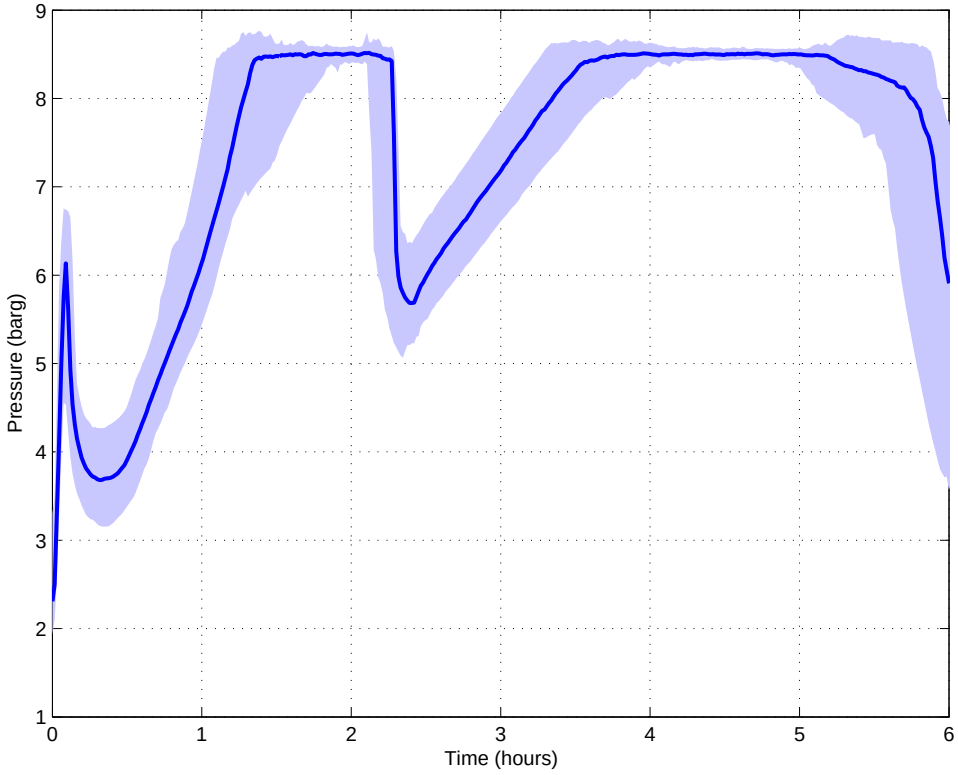

Figure 3.2: Empirical pressure profile. The shaded area represents the area between the 5$^{\text{th}}$ and 95$^{\text{th}}$ percentile

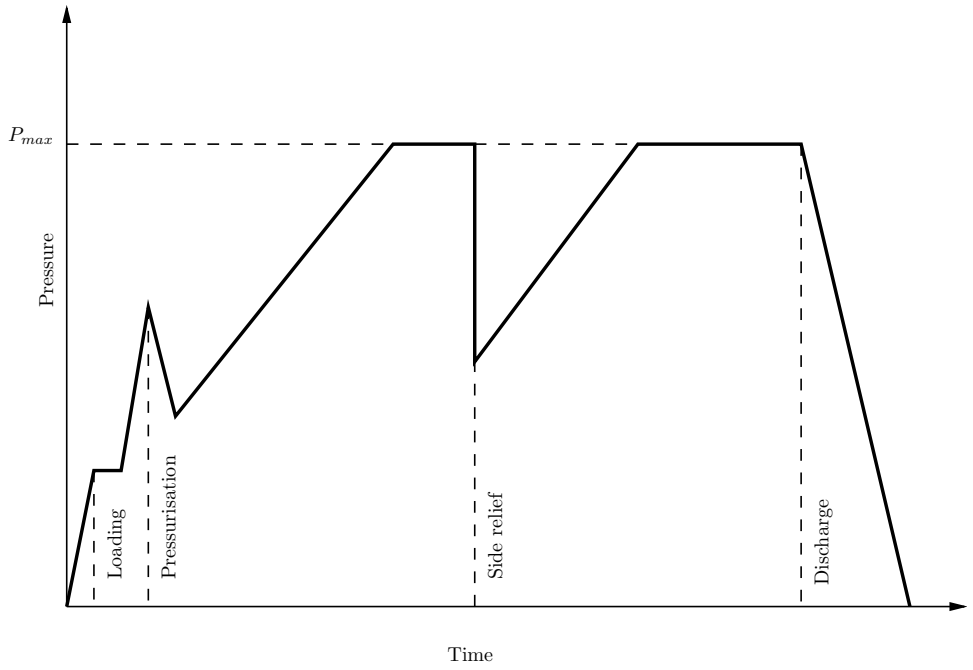

Figure 3.3: Pressure profile

3.6.4 Heating

After loading and pressurisation, the liquor is heated using steam fed to the external heat exchanger. Figure 3.4 shows the median temperature profile for 300 cooks in 2003. The shaded band represents the area between the 5^{th} and 95^{th} percentile.

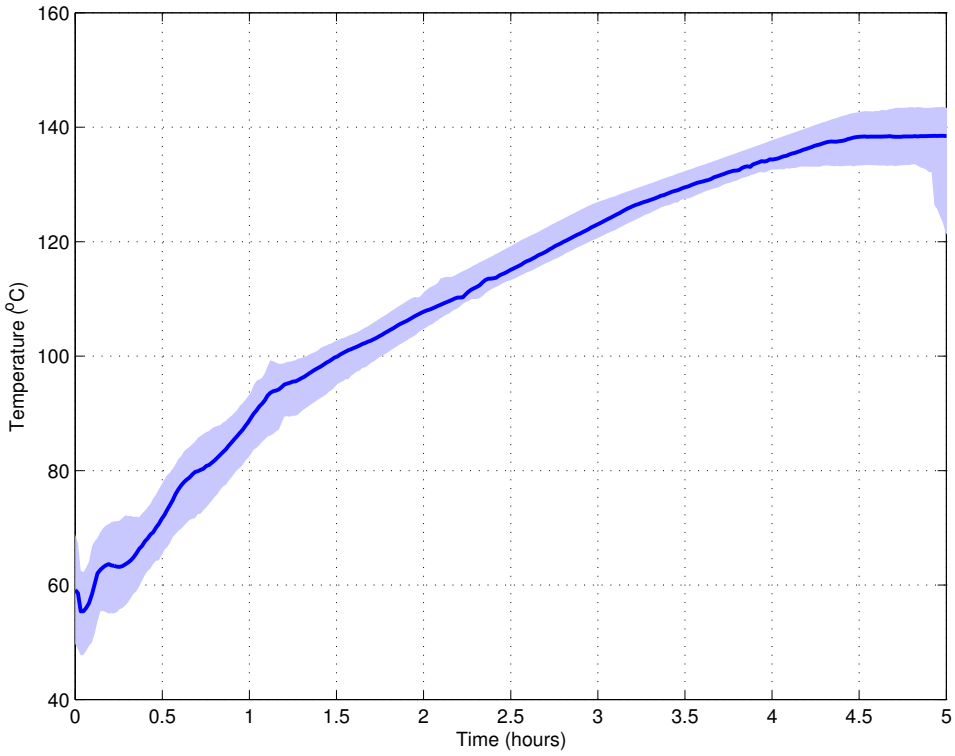

Figure 3.4: Empirical temperature profile. The shaded area represents the area between the 5^{th} and 95^{th} percentile

Several phases of heating of the digester can be distinguished. To clarify the significance of each stage, figure 3.5 shows an idealised temperature profile, similar in shape to the empirical profile in figure 3.4. Slopes and time intervals have been exaggerated for clarity. The heating phases are described below:

Smooth steam ramp The steam valve is opened in a ramp to a set valve position. The first 40 minutes of heating is known as the smooth steam ramp. During this time, the steam valve is ramped to a set valve position in a pre-set time, irrespective of the starting cook temperature. This ramp time is 40 minutes on the calcium digesters and 30 minutes in the magnesium digesters. The steam flow during this time is variable, since all of the digesters draw steam from a common steam line. The steam demand of the other digesters will influence the amount of steam available to a specific digester. The steam flow can be up to 15 tons per hour, but is usually closer to 10 tons per hour.

Rise to T_A The next heating phase heats the liquor to a temperature of T_A. A fixed rate

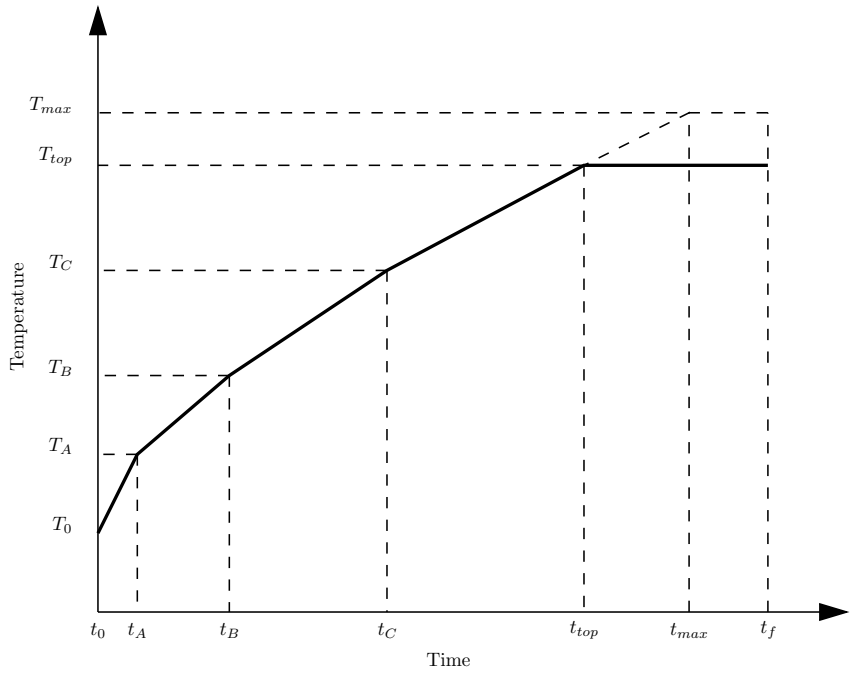

Figure 3.5: Idealised temperature profile. Slopes and time intervals have been exaggerated for clarity

for the rise in temperature is calculated from the temperature at the start of the cook and the time allowed for this phase. From the slope of this temperature line, a continuous setpoint temperature can be calculated in order to control the steam supply to the heat exchanger. The control of the temperature is based on the top temperature, measured at the end of the circulation line. Normal feedback control on the rate of steam addition is used, based on the measured top temperature and the calculated setpoint temperature (see figure 3.1).

The set time for this phase is approximately 90 minutes.

Rise to T_B As soon as the temperature reaches T_A, the temperature is ramped up to T_B similar to the previous ramp.

Rise to T_{max} The control algorithm calculates the desired top temperature in order to reach the setpoint value for the degree of polymerisation. A similar control formula to the one used for the T_A temperature rise is used to calculate the setpoint temperature during this phase. Once the desired maximum temperature has been reached, the setpoint temperature is fixed at this maximum temperature for the rest of the cook.

When the temperature of the liquor in the top of the digester has reached T_A, some of the liquor in the digester will be let out. This is known as side relief. The side relief will drop the level in the digesters to 10,5 m for the calcium-based digesters and 8,9 m for the magnesium-based digesters. This will also cause the pressure to drop significantly.

However, the pressure isn't raised to the maximum temperature, but is allowed to climb gradually as temperature increases. Once the pressure has reached its maximum value of 8,2 bar, it will be controlled again at this value.

When the specified cook time has been reached, the liquor circulation will be stopped. Some of the liquor will be discharged and the pressure will drop to about 600 kPa_g. When the pressure has reached 600 kPa_g, the high-pressure gas release will start. During this phase, the pressure in the digester is relieved in a controlled manner by opening the high-pressure gas release valve from fully closed to fully opened in a set time. When the pressure reaches 350 kPa_g, the low-pressure gas release phase will be started and the pressure will be dropped to atmospheric pressure. The pulp is then discharged and conveyed to the next phase of the total operation.

3.7 Control System

An ABB DCS system is installed on the plant and controls several of the variables discussed in section 3.6. The exact working of the control system is complex and will not be discussed here. However, several points of control system operation are important in understanding the problem addressed in this dissertation and will be discussed in chapter 4.

CHAPTER 4

Control analysis

This chapter analyses the control problem. The problem is divided into relevant time frames and the per-cook frame is shown to be relevant to the design. From this, the controlled variable and possible manipulated variables are isolated. Other pertinent variables which influence the process are also identified and explained.

4.1 Control time frames

Control time frames are an important aspect of layered control systems. Paragraph 2.2 and the control triangle in figure 2.2 cover this concept in more detail.

Control of the digester takes place in three different time frames. The first is the *continuous* time frame. Control on this level involves keeping the top temperature ($T_{m,\ top}$) on a temperature setpoint. Control of the final DP takes place *per cook*, representing the second time frame, while the final DP must be kept on target through a number of cooks (*N cooks*), taking into account long-term changes in the process. This long-term optimisation takes place in the third time frame. The second and third time frames both encapsulate discrete control problems with small sampling rates.

To illustrate the time frames in question, they will be discussed separately in the following sections. In the diagrams to follow, increased sampling frequency is indicated by thicker lines connecting units.

4.1.1 Continuous temperature control

Figure 4.1 shows the temperature control loop on the digester. This control configuration is also indicated in the digester schematic in figure 3.1 and corresponds to the normal feedback controller setup as shown in figure 2.4.

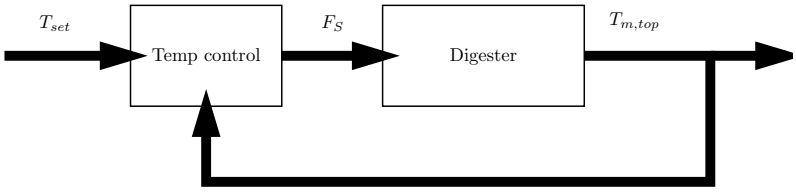

Figure 4.1: Continuous time frame: Low level temperature control loop

The temperature in the digester is controlled by manipulating the steam flow rate to the external digester. This first level of control is already handled satisfactorily by the feedback controllers on each digester (Meneghel, 1998b).

4.1.2 Per cook DP control

The temperature setpoint for the low level temperature control system is supplied by a profile generator which ensures that the predefined temperature profile (as shown in figure 3.5) is followed. The profile generator requires the value of T_{top}, the constant top temperate for the cook, in order for it to generate a complete profile. Figure 4.2 shows how the value of T_{top} influences the final DP of a cook.

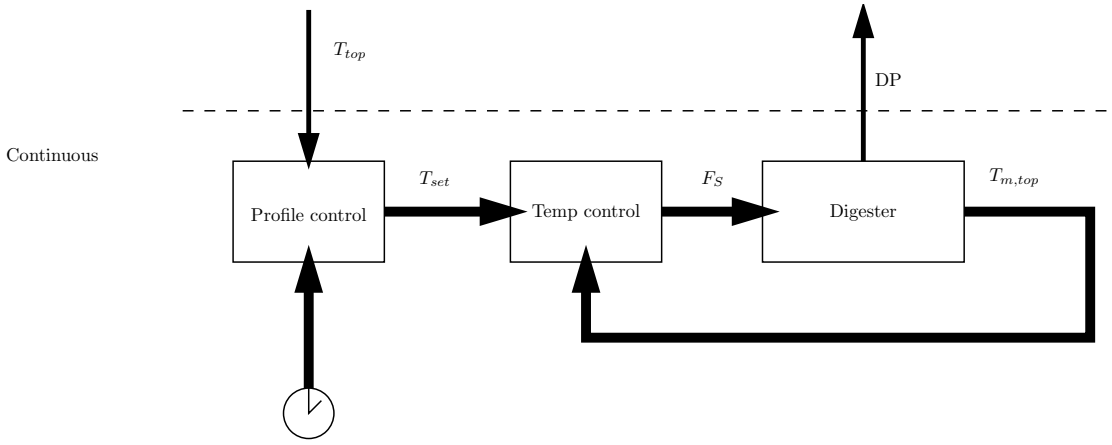

Figure 4.2: Per cook time frame: DP control. Notice that the continuous time frame shown in figure 4.1 is included below the dashed line.

As can be seen from figure 4.2, the final DP of the cook is determined by the temperature profile that the digester is taken through. Even though the profile generator determines this profile, the value of T_{top} is specified externally. It should be clear that the value of T_{top} therefore determines the value of the final DP to a great extent.

4.1.3 N cook time frame

The results of a number of cooks are collected using a historian system. These stored results can be analysed to check the performance of the system over time. New model

parameters can also be passed to the DP controller so that long-term changes in plant behaviour can be accommodated. The diagram shown in figure 4.3 shows the inputs and outputs of the N cook time frame.

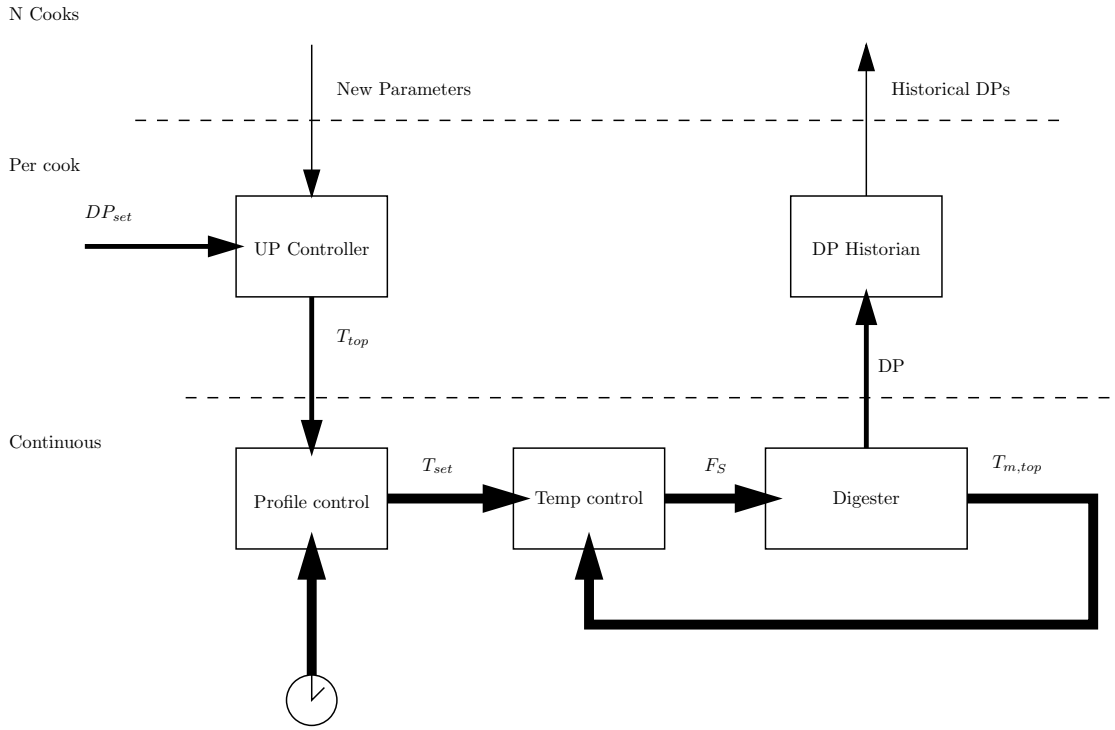

Figure 4.3: All time frames, including N cook optimisation. Note that the normal operation of each cook as shown in figure 4.2 is included below the upper dashed line.

In this time frame, the controller responsible for outputting the correct value of T_{top} to the profile generator is shown. This is the UP controller. The model parameters used in the controllers are changed every N cooks, placing this update in the N cooks time frame. It should be borne in mind that the controller reads process variables from the plant with other sampling frequencies as well. Figure 4.3 is intended to show the position of the controller in the time frames, but this is by no means a unique representation.

4.2 Controlled variable

The main controlled variable is the DP, as described in paragraph 3.5.1. On-line measurement of the DP on the plant is not currently an option. The DP of the pulp sampled after a cook is measured off-line using the cuprammonium test as described in paragraph 3.5.3. Measurement of the DP takes approximately 2 hours, at which time this value is entered on the site database and can be accessed by the control program.

From this information and with reference to figure 4.2, it is clear that the DP is a *per cook* variable. The controller will therefore operate in the per cook time frame.

4.3 Controller output

The only variables on the digester that can be manipulated continuously are the steam flow to the digester and the pressure release valve position. However, the temperature profile is specified by the heating procedure as described in paragraph 3.6.4 and the pressure is determined predominantly by the temperature of the digester.

Referring to figure 3.1 as well as figure 4.1, the low-level control system can be seen to mask the steam flow rate as a variable in a cascade control system.

This means that the desired controller output is T_{top}, the temperature reached during the constant top temperature phase. Refer to the temperature profile presented in figure 3.5 for more details. T_{top} is input per cook, and therefore is the controller output of the controller shown in figure 4.2.

4.4 Disturbance variables

The following possible disturbance variables were identified by Kilian (1999):

Wood load Historical data collected over a one and a half year period show that the wood load per batch varied between 90 and 120 tons and that the standard deviation of the wood load was 6 tons (Pellow-Jarman, 1997). This could be due to several factors including:

- The wood density
- The chip dimensions: The average chip size is difficult to control, since no continuous measurement of the chip size is possible. Various factors during chipping can lead to varying chip sizes.
- The packing of the chips and the amount of steam flow to the Svensson packers: The efficiency of the packing of the wood chips will depend largely on the steam pressure and thus the amount of steam flow to the packers.

Liquor load Internal investigations at Sappi Saiccor showed that the liquor level usually drops between zero to two meters after the loading has been completed (Meneghel, 1998b). The historical data show that the liquor load has varied between 172 m^3 and 263 m^3. The standard deviation was 10 m^3 over this period. This variability is dependent on channelling and air pockets in the digester after wood loading. It was also indicated that the method of measuring the liquor level wasn't very accurate. The reason for this is that the bottom impulse line for the level measurement is situated at the bottom of the digester in the same area as the entry of the liquor loading line. When liquor loading is started, the impulse line is falsely pressurised

and the level indicator gives a level reading that is higher than the actual level. (Meneghel, 1999)

Starting temperature The initial temperature of the liquor will depend largely on the ambient temperature. The effect of this will be that a fixed temperature ramp cannot be used, but that the rate of the temperature rise must be variable to obtain a specified temperature at a certain time.

Liquor strength Variations in the liquor composition at the start of the cook will influence the pH of the liquor. The variability in the starting liquor composition is apparently largely due to operator error during liquor analysis and a dilution system based on flow and not composition (Meneghel, 1999). The CaO content of the liquor loaded into the digester can vary between 0,7% and 1,28%. The amount of wood loaded into the digester also depends on the liquor strength. Therefore, the variability of the liquor strength will cause great uncertainty about the initial conditions and will necessitate a model that can be changed to represent the starting conditions.

Circulation flow The flowrate of the circulation stream is not controlled and is governed by the resistance to flow in the line. Long-term scaling of the circulation return line, as well as clogging of the extraction line during a cook, cause changes in the flow that are difficult to predict and which cannot be controlled. The temperature profile through the digester is determined by the circulation flow and deviations in the flowrate can influence the product quality if the control strategy does not compensate for it.

4.5 Constraints

4.5.1 Safety

For safety reasons, the pressure in the vessel has to be kept below 8,4[barg]. The controller does not have to make provision for this limit, as the pressure profile is dependent on the temperature profile and kept on the safe limit by a pressure release valve.

4.5.2 Product quality

The rate of change of temperature over time must be controlled during the first stages of the cook. When the temperature is raised too fast, SO_2 penetrates the chips rapidly, leading to condensation inside the chips. This in turn causes areas of high acidity, which leads to a 'burned' cook.

4.5.3 Hard constraints

The rate of heating of the digester is constrained by the heat transfer possible in the heat exchanger. Due to the design of the exchanger and the steam available, the temperature increase is limited to roughly 3,75℃/hr.

There is also a maximum temperature of 145℃ set for the digester.

4.6 Summary

An initial guess of the control structure is shown in figure 4.4. This figure is intended to

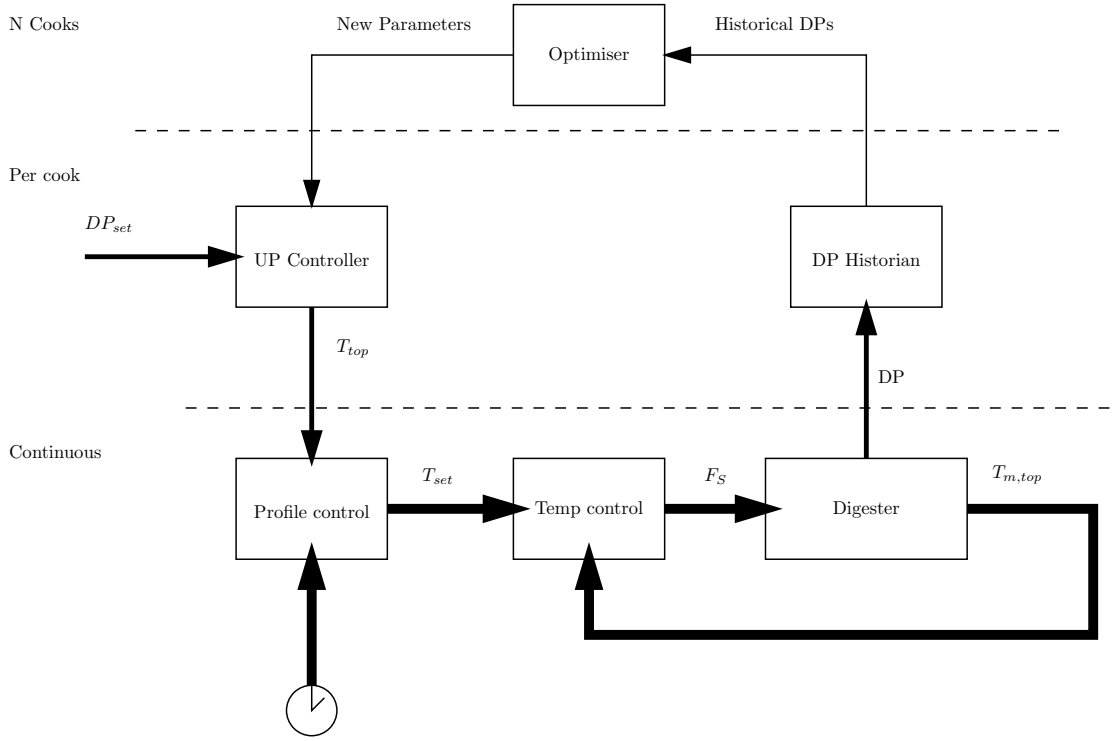

Figure 4.4: Initial guess of the complete control structure

show the components necessary for the control of DP in an initial structure.

The controlled variable is the final DP of the discharged pulp. The controller should will output a value for T_{top} to the profile controller which will output a temperature setpoint to the temperature controller and control the digester along the predetermined profiles.

Ultimately all control action is implemented by manipulation of the steam flow rate, but the low level control systems in place to control the temperature profiles are working well enough so that the controller just has to concern itself with determining the optimal top temperature that will result in the correct DP being obtained. Detailed development of the controller is covered in chapter 6.

CHAPTER 5

Current development

This chapter describes the current control structure in place on the plant, as well as progress that had been made before the new controller implementation was started. It involves the derivation of a valid model of the reactor and preliminary analysis of the control problem as proposed by Kilian (1999). The current controller is based on a model called the S-Factor, using an empirical 'target factor', which is set equal to an integral of the lignin reaction rate during the cook. The UP model uses a more involved set of equations with less simplifying assumptions combined with a direct numerical solution of the optimal maximum temperature which will reach the DP setpoint.

The current performance measures in use on the plant are also discussed critically, and a change in this, as suggested by Kilian (1999), is mentioned as a partial solution.

5.1 S-factor model

5.1.1 Description

The description of the S-factor model is taken largely from Kilian (1999). The model is derived from a delignification rate equation first proposed by Yorston & Liebergott (1965) based on an assumed correlation between the lignin content of the solid phase in the reaction and the pulp viscosity. The delignification rate equation in the form also later reported by Hagberg & Schöön (1973) is given here:

$$-\frac{\mathrm{d}[L]}{\mathrm{d}t} = K_L(T) \cdot [L]^a \cdot \left\{ \left[HSO_3^- \right] [H^+] \right\}^n \tag{5.1}$$

Yorston & Liebergott determined that this equation could be expressed in terms of more easily measured qualities. n was also found to be equal to 0,75. The restated rate equation is

$$-\frac{\mathrm{d}[L]}{\mathrm{d}t} = K_L(T) \cdot [L]^a \cdot \{P_{SO_2}\}^{0,75} \tag{5.2}$$

The partial pressure of the SO_2 is determined by assuming equilibrium between the dissolved SO_2 and the SO_2 in the space above the reaction mixture. Further, it is known that the temperature dependence of the rate $K_L(T)$ is described by the Arrhenius equation in the form shown in equation 5.3

$$K_L(T) = A_0 e^{\left\{B-\left(\frac{E_0}{RT}\right)\right\}} \tag{5.3}$$

The factor B is known as the normalisation factor. It is used to normalise the equation to 100℃. Integrating the rate equation in equation 5.2 and assuming that the order of the reaction is unity ($a = 1$) gives the "S-factor" equation:

$$SF = -\int_{L_0}^{L_f} \frac{1}{A_0[L]}\mathrm{d}[L] = -\int_{t_0}^{t_f} \exp\left\{B - \left(\frac{E_0}{RT}\right)\right\}\mathrm{d}t \tag{5.4}$$

Integration of the left-hand side of this equation yields:

$$[L_f] = k_1 e^{\{-A_0 \cdot SF\}} \tag{5.5}$$

By assuming that the viscosity is proportional to the lignin content of, viscosity can be calculated in the same way, with a different proportionality constant:

$$\mu = k_2 e^{\{-A_0 \cdot SF\}} \tag{5.6}$$

The assumption of linear dependence of viscosity to lignin content is the main weakness of the model and many mills have adapted this basic formula to fit the data gathered from their plants.

5.1.2 Local modifications

Sappi Saiccor came to the conclusion from their own studies that it would be more accurate to use the actual SO_2 concentration of the liquor instead of the partial pressure of the SO_2 (Meneghel, 1999). Equation 5.4 was adapted as follows:

$$SF = -\int_{L_0}^{L_f} \frac{1}{A_0[L]}\mathrm{d}[L] = -\int_{t_0}^{t_f} \exp\left\{B - \left(\frac{E_0}{RT}\right)\right\}\left(SO_2^{free}\right)^n \mathrm{d}t \tag{5.7}$$

As can be seen from the above equation, the model was initially based on the free SO_2 concentration. However, SO_2 can also be present as combined SO_2 in the form of bisul-

phite, which complicated the measurements.

The use of the direct measurement of the SO_2 concentration instead of the partial pressure made the S-factor directly dependent on the base concentration in the liquor. The relationship between the base concentration and the target S-factor was determined to be non-linear. This lead to the development of the following model, which is currently in use:

$$SF_{target} = A \times [SO_2^{free}]^2 + B \times [SO_2^{free}] + C \times (\%Base) + D \tag{5.8}$$

where A, B and C are all constants determined from plant data and D is a constant which is updated continuously by means of a feedback system. The constants A to C were calculated for different wood species and can be changed when new wood species are used. The feedback system compares the target final degree of polymerisation after each cook with the actual value obtained when the cook was controlled using the S-factor model. Some adjustments are then made to the constant D to try and make the model more accurate.

5.2 Current control structure

5.2.1 Continuous control

To ensure that $T_{m,\ top}$ is kept on the profile shown in figure 3.5, a simple feedback structure is used to manipulate the steam flow rate to the external heat exchanger. Temperature control has been shown to be quite efficient except under circumstances where the other digesters' steam requirements are high and cause the temperature to lag behind setpoint during the high temperature part of the profile.

5.2.2 Per-cook control

The setpoint for the temperature controller is output by a higher level control system, following a profile which changes with every cook. The basic shape of this profile is as shown in figure 3.5.

The S-factor model discussed above is used to determine the process path, based on the measurement of the initial conditions, that must be followed in order to achieve the desired final specifications of the pulp. Due to process constraints, the profiles used for the temperature and pressure are quite rigid (as shown in paragraph 3.6), with the only true variable being the maximum temperature in the final temperature ramp.

Control strategy

The following control strategy is used to implement the S-factor controller. (ABB, 1994):

1. Equation 5.8 is used to calculate a target S-factor based on a liquor sample taken one hour after the start of the cook. This test is known as the *one-hour test*, and provides the concentrations of SO_2 and CaO in the liquor at the time of the test.

2. To find the temperature that will satisfy equation 5.4, the right hand side is integrated numerically. Assuming that no reaction takes place below T_B, the system waits until the temperature reaches this point before starting to sum the rate given by equation 5.7. Internal investigations resulted in the value of n in this equation being set to zero and thus effectively removing the dependence of the model on the free SO_2 concentration. The following rate equation resulted (ABB, 1994):

$$r = \exp\left\{B - \left(\frac{E_0}{RT}\right)\right\} \tag{5.9}$$

   The system checks at each time step whether if the target S-factor would be reached if the current temperature were maintained for the rest of the cook stages. In other words, the current temperature will be the highest temperature reached (T_{top}), if the calculations show that the target will be reached. The temperature is not allowed to go above T_{max}.

3. A sample of the discharged pulp is taken to the plant laboratory for analysis. The actual DP reported by this analysis is entered into a database to allow trending and quality control. This measurement takes place once for each cook.

4. Using a local technique, plant personnel change the value of D in equation 5.8 in an attempt to achieve better control. Additionally, operators may choose to modify the target as the cook is progressing in order to provide quick response to perceived trends due to wood composition and other factors not modelled by the S-factor equation.

5.2.3 Problems

Studies done on historical data show that the performance of the S-factor model is not satisfactory (Meneghel, 1998a). Several issues have been identified concerning the use of the S-factor model for control. The model itself poses the following problems:

- The assumptions regarding the reaction rate render the model linear with respect to many of the inputs. This affects the ability of the model to perform adequately when the process conditions change.

- Assumptions about the SO_2 concentration are not very accurate. The dissolution of the dissolved SO_2 is not modelled.

The inadequacies of the model lead to inadequate control. In practise, the controller based on the S-factor model will also be less efficient due to the parameters used in determining the S-factor target.

The value of the tuning parameter D has only the qualitative relationship that lowering the D value will increase the viscosity of the pulp and vice versa. There is difficulty in determining the value of D preemptively given a change in wood composition, liquor strength and many other factors unmodelled by the S-factor model.

5.3 UP model

Kilian (1999), in the initial work of the controller project, derived a more complete model of the reactions in the digester. This model can be summarised by the following assumptions:

1. The reactions in the digester can be accounted for by modelling the rate of cellulose degradation, lignin dissolution and strong acid equilibria in the digester.

2. The temperature and pressure of the vessel are known.

3. The initial composition of the reaction mixture is known from a test of the liquor.

5.3.1 Variables

Table 5.1 shows the variables used in the equations that make up the UP model. There are a total of 15 variables. The next section shows that there are enough equations to solve for all the variables.

5.3.2 Equations

To model the rates of the chemical reactions inside the digester, the following reaction rates are used:

$$-\frac{\mathrm{d}[L]}{\mathrm{d}t} = k_L[L]^a \cdot [HSO_3^-]^\alpha \cdot [H^+]^\beta \tag{5.10}$$

$$-\frac{\mathrm{d}[SA]}{\mathrm{d}t} = \frac{k_{SA}}{\nu} \cdot [SA^-]^n \cdot ([L]_0 - [L])^m \cdot [HSO_3^-]^b \cdot [H^+] \tag{5.11}$$

$$-\frac{\mathrm{d}[C]}{\mathrm{d}t} = k_C[H^+]^\delta \tag{5.12}$$

The temperature dependence of all the k factors above can be described by the Arrhenius relationship $k = k_0 \exp(-E/T)$, with E and k_0 known for each of these reactions.

Table 5.1: Variables used by the UP model (Kilian, 1999)

			Typical range	
Variable	Symbol	Units	Low	High
Wood constituents (2)				
Residual Lignin Concentration	$[L]$	mass %	0	30
Cellulose Concentration	$[C]$	kmol/m^3	300	2 100
Liquor Composition (3)				
Sulfite concentration	$[HSO_3^-]$	kmol/m^3		
Hydrogen ion concentration	$[H^+]$	kmol/m^3		
Strong acid concentration	$[SA^-]$	kmol/m^3		
Digester conditions (2)				
Temperature	T	K	288	423
Pressure	P	Pa$_a$	103	940
Equilibrium variables (4)				
Partial pressure of SO_2	p_{SO_2}	Pa	700	940
Partial pressure of water	p_{H_2O}	Pa	0	240
Dilution constant of SO_2	K_{SO_2}	kmol/m^3		
Vapour-liquid equilibrium constant	K_P	(kmol/m^3)^2/Pa		
Per-cook variables (4)				
Combined SO_2	*combined* SO_2	kmol/m^3		
Free SO_2	SO_2^{free}	kmol/m^3		
Total positive charge	$[M^+]$	kmol/m^3		
Specific volume of liquor	ν	m^3/kg	0,9	1

Liquor composition is modelled by equilibrium equations for the SO_2 concentration in the liquor and vapour pressure in the space above the reaction liquid.

$$K_{SO_2} = \frac{[H^+][HSO_3^-]}{[SO_2]} \tag{5.13}$$

$$K_P = \frac{[H^+][HSO_3^+]}{p_{SO_2}} \tag{5.14}$$

Both of these factors are temperature dependent. The temperature dependence can be calculated by substituting known values of B and C in the Antoine equation shown in equation 5.15 and solving for A:

$$\log_{10} A = B + \frac{C}{T} \tag{5.15}$$

In addition, the metal ion concentration can be modelled using electron-neutrality arguments as shown in the following two equations

$$\left[M^+\right] + \left[H^+\right] = [HSO_3^-] + [SA^-] \tag{5.16}$$

$$\left[M^+\right] = 2 \cdot [combined\ SO_2] \tag{5.17}$$

The total pressure in the space above the reaction liquid is calculated as the sum of the partial pressures of the SO_2 and the water as shown in equation 5.18

$$P = p_{SO_2} + p_{H_2O} \tag{5.18}$$

The three rate equations, two equilibrium equations, two electron-neutrality equations and one total pressure add up to eight equations. Two temperature dependent equilibrium constants can be calculated from parameters in the shape of the Antoine equation shown in 5.15, giving ten equations. As there are 15 variables, this leaves five variables to be specified.

The temperature and pressure are read from the environment during a cook and specified by approximations during the simulation. At the start of a cook, the liquor-to-wood ratio is known and the free and combined SO_2 concentrations are read during the one-hour test. Specifying these five variables completely specifies the problem.

5.4 Current performance measures

5.4.1 Coefficient of variance

The coefficient of variance is the current measure of performance on the Sappi Saiccor. The COV is calculated for a subset if cook data. The formula used is given in equation 5.19

$$\mathrm{COV} = 100 \times \frac{\sqrt{\frac{1}{n-1}\sum_{i=0}^{n}(\mu_i - \bar{\mu})^2}}{\frac{1}{n}\sum_{i=0}^{n}\mu_i} \tag{5.19}$$

This equation has a disadvantage as a long-term performance measure, as it does not take into account that the target viscosity changes with time. This is analogous to 'aim' and 'grouping' in target shooting. The COV only checks grouping. All the cooks might have good grouping, but they would still not be on target.

A modified COV was therefore proposed by Kilian (1999) that would take this into account. The target viscosity instead of the average is used, leading to equation 5.20.

$$\mathrm{COV}_{\mathrm{target}} = 100 \times \frac{\sqrt{\frac{1}{n-1}\sum_{i=0}^{n}(\mu_i - \mu_{target})^2}}{\frac{1}{n}\sum_{i=0}^{n}\mu_i} \tag{5.20}$$

It can easily be seen that this makes comparison of performance possible over a larger period of time – not only where the target remained equal to the average of the viscosities obtained.

CHAPTER 6

Controller design

This chapter explains the design of an improved controller for the pulp digester. It covers conceptual design work and theoretical justification of this design as a variation on well-documented designs from literature. Included in the design are methods to provide feedback using on-line tuning.

6.1 Conceptual design

6.1.1 Controller

From chapter 4, it should be clear that it is not possible to use the final DP for normal feedback control during the same cook, as the measured value only becomes available after the cook has finished. The problem is the discontinuous nature of the digester output. In fact, any control scheme that relies on the DP to be roughly continuous will be at a disadvantage.

The DP changes due to many factors which can only be properly evaluated with the help of an accurate model of the system. Knowing that the outcome of a cook can only be reliably evaluated using the inputs for that specific cook leads to the choice of a feedforward type controller for the per-cook time scale (refer to figure 4.2 to see how the plant is defined for this time frame).

6.1.2 Feedback

Even though the controller can not respond purely on the measured DP for a certain cook, this information is obviously important. Ideally, some mechanism should be incorporated which ensures that the measured DP is indeed on target. The information obtained from the results of several cooks should be used to avoid the problem of discontinuous outputs

and once-off problems. Ideally, the model used by the feedforward controller should be conditioned so that the best accordance between the model and the real process is obtained. This conditioning can be obtained by periodically modifying the model parameters.

6.1.3 Concept summary

An overview of the controller structure that is required is shown in figure 6.1. Note that this figure does not indicate sampling rates of the signals, but that the model parameter adaption mechanism operates in the N cooks time frame.

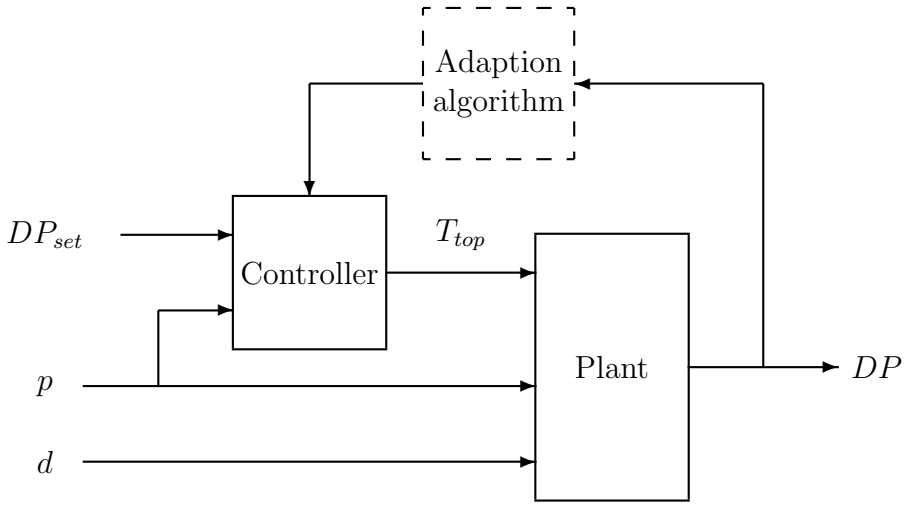

Figure 6.1: Overview of controller structure

The controller reads several process variables p and predicts the top temperature, T_{top}, for the cook that will result in the correct DP. Clearly, some disturbance variables, d, enter the process that affect the result of the cook but are not measured.

6.2 Theoretical justification

6.2.1 Controller

The controller shown in figure 6.1 reads process variables and a DP setpoint and is required to return T_{top}, which is input into the digester system. The relation between DP and T_{top} in the controller is clearly the inverse of the relation in the digester. In other words, the controller should use the process variables it reads to construct an inverse of the digester process. This corresponds well to the classical feedback controller in section 2.3.4, except that the inverse is constructed using additional information about the process variables.

6.2.2 Adaption

The adaption mechanism just described in section 6.1.2 resembles the self tuning adaptive control structures described in section 2.6.3. The synthesis of the controller described in that section corresponds to the production of new controller parameters in the proposed scheme. It is however important to note that the time frame proposed for the parameter adaption is different from that of the control action.

6.2.3 Summary

The proposed structure conforms well to existing theory, especially the self tuning adaptive controller discussed in section 2.6.3, generating a feedforward type controller as discussed in section 2.3.4. Similar control structures have been employed successfully in many instances. This indicates that the controller structure is a valid proposal.

6.3 Algorithm

The controller described in the above sections is implemented using the following algorithm:

- Initial model parameters are loaded from a file. The model parameters stored in file are listed in appendix A.
- The program reads status information from the plant, waiting for a cook to start. The database system stores a state tag which is read to determine whether a cook has started.
- As soon as the start of a cook has been detected, the controller reads plant data and stores the information internally. Note that no simulation is done in this phase, as the initial conditions for the integration of the model equations are only available after roughly an hour, once the analysis of the liquor sample as been done (see section 5.2.2).
- As the program reads data from the plant, it checks whether the results of the one-hour test have become available. This test supplies the liquor composition at the time of the test.
- When the one-hour test results are available, the controller program simulates the cook up to the current point in time using the stored process variables and initial values calculated from the test results. The simulation is done by integrating the three differential equations mentioned in section 5.3.2 and solving the remaining equations to yield all the variables listed in table 5.1.

- The program then simulates reactions inside the digester in real time using the same equations, incorporating real time values of the process variables (temperature, pressure and the flow through the heat exchanger) that are available from the plant database system.

- When the temperature reaches T_C, the program starts an optimisation routine that simulates the remainder of the cook using the current states as the initial conditions for each trial cook. The optimisation finds a value for T_{top} that will minimise the viscosity error at the end of the cook.

- This temperature is displayed on the screen for entry by an operator into the plant control system. The plant control system uses this value to ensure that the temperature is ramped up to T_{top} in the required time.

- The previous two steps are repeated 5 minutes after the first prediction to verify the correct operation of the predictor.

- The model equations are integrated up to the end of the cook.

- In intervals of ten cooks, the data for the last ten cooks are read from the plant database, and a separate optimisation process is initiated to reduce the error between the measured DP and the DP predicted by the model for each of these cooks.

This control strategy is shown in a flow diagram in figure 6.2.

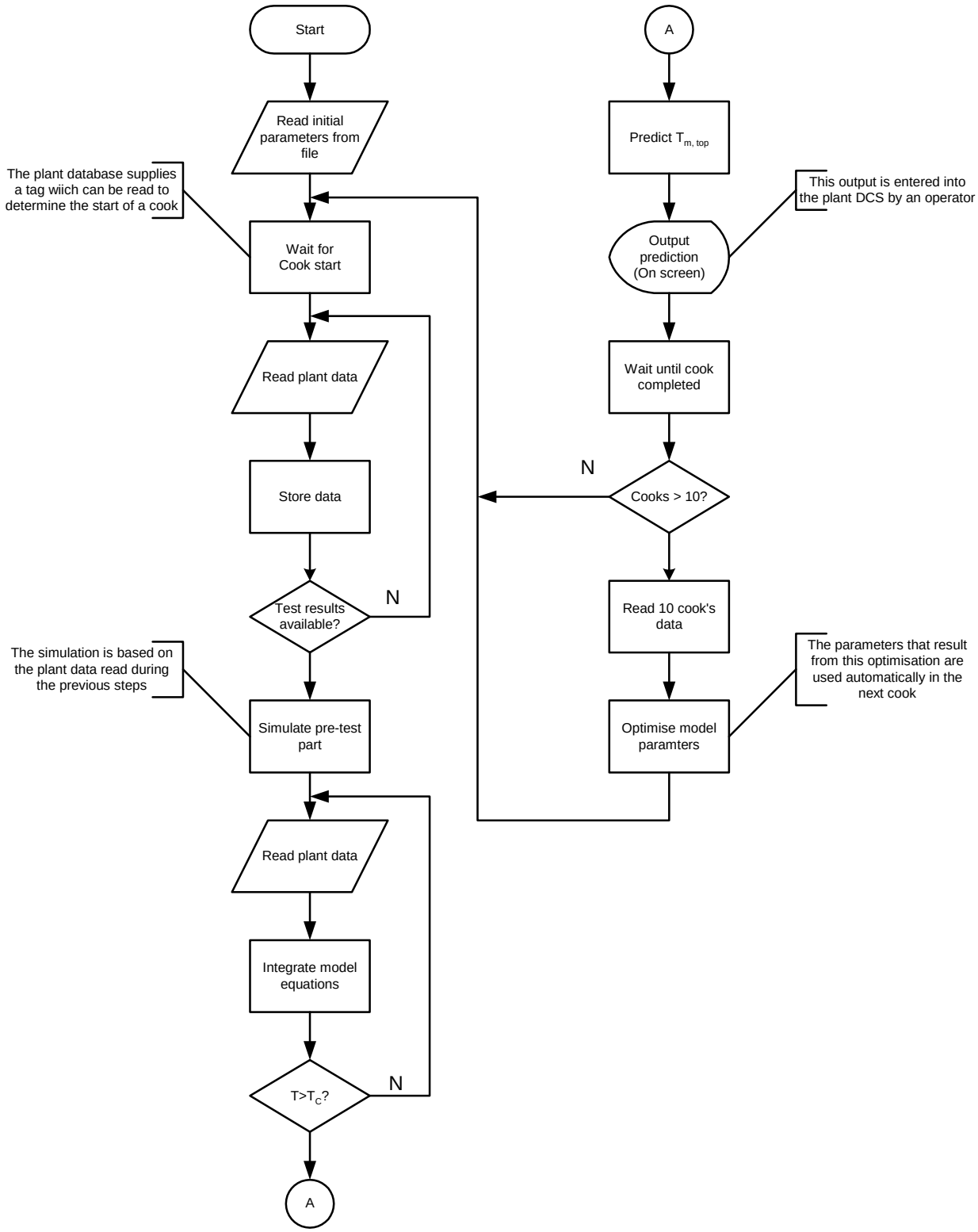

Figure 6.2: Control strategy flow diagram

CHAPTER 7

Monte Carlo Modelling

The S-factor controller is to be compared with the UP controller by modelling the control action of both on a modelled digester described by a valid model as proposed by Kilian (1999). This digester is subjected to random inputs generated to conform to predetermined distributions and the control performance of both algorithms is evaluated. The methods described in this chapter will yield the theoretical results that are to be used as a measure of the theoretical performance of the different control strategies and the benefits realisable by implementing the UP controller.

7.1 System overview

As discussed in section 2.10, Monte Carlo simulation requires known input distributions and a system model to be used in the simulation. Building on the analysis of chapter 4, the system that is to be modelled can be described. The model must be built to incorporate all three of the time frames identified in the analysis.

It can be seen from figure 7.1 that the system model consists of the digester model and the controller. The physical digester is modelled using the equations discussed in section 5.3. In the real world, the physical digester is controlled by a DCS system installed on it. This DCS system is responsible for the control of the digester temperature as well as ensuring that the digester goes through all the phases required by the cooking recipe. These phases were discussed in detail in section 3.6. For the simulation to be an accurate portrayal of reality, action of the DCS has to be simulated as well. The combination of the DCS and the reaction model is referred to as the 'digester model'. The digester model corresponds to the plant used in the controller design discussed in chapter 6, also corresponding to the per cook time frame discussed in section 4.1.2.

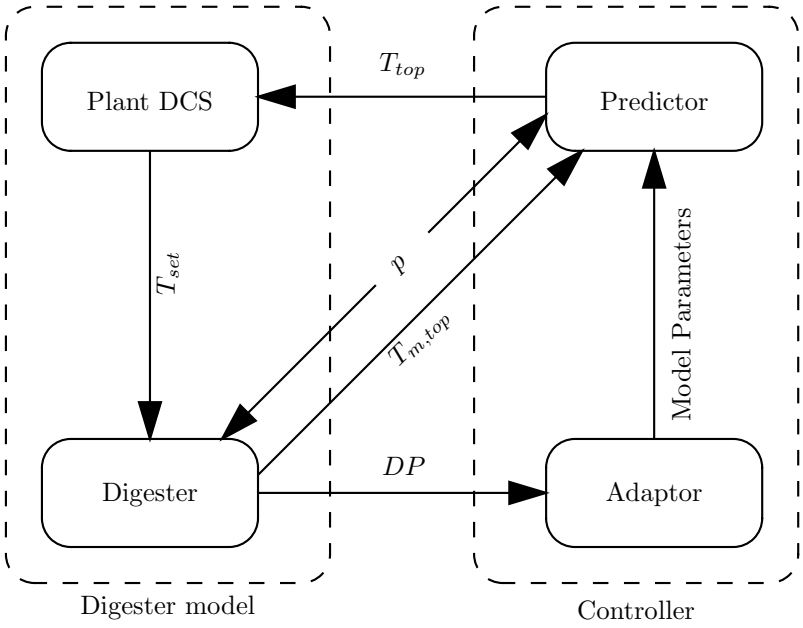

Figure 7.1: Schematic representation of the system modelled during Monte Carlo simulation

The controller that specifies the value of $T_{m,top}$ for the digester model as well as the adaption mechanism that adapts the model parameters to reflect changes on the plant is referred to simply as the 'controller'.

In addition to the variables already discussed in detail in other sections (the DP and temperatures), the model used for the Monte Carlo simulations has to take into account the many variables that affect the final DP on the real digester. These variables are grouped into a vector of process variables, p, on the diagram in figure 7.1 and are the same as p mentioned in section 6.1.3. How the values of these variables are determined will be discussed shortly.

7.2 Input model

In order to model a complete cook, the conditions experienced by a real digester must be simulated. The simulation uses two classes of input variables: those that stay constant for the duration of the cook, and those that vary during the entire cook.

7.2.1 Constant inputs

The values of these parameters stay constant during the cook, but may vary from cook to cook. The digester model parameters were kept constant during a cook using the parameters obtained by (Kilian, 1999). The parameters that were used are listed in appendix A.

7.2.2 Continually variable inputs

Three continually variable inputs are modelled: the temperature and pressure profiles and the side circulation flowrate. Because the UP controller and the S-factor controllers have different ways of specifying their control output, the S-factor controller algorithm was modified slightly to allow the temperature profile to be modelled in the same way for both controllers.

The S-factor controller uses a value for T_{top} specified along the slope that goes to T_{max}. Refer to figure 3.5 to see this temperature profile. The UP controller algorithm does not have the same slope constraint, but it was introduced to ease the implementation of the controller on the plant.

The pressure profile on a real digester is dependent on the temperature of the digester and the pressure added during the pressurisation stage. The equations to model this dependence were not used. Instead, a fixed pressure profile very similar to the one shown in figure 3.3 was obtained by averaging the pressure profile for several cooks.

This simplification can be justified when considering that the pressure is affected most at high temperatures. The high temperature phases of the cook correspond to the times when the pressure is being kept at the maximum pressure by the pressure release system. Therefore, there is very little variation in the pressure profile from cook to cook. The assumption reduces computational complexity of the Monte Carlo problem, and allows the same models used for the *in-situ* controller to be used without modification.

All values are assumed to interpolate linearly between the given turning points on the profiles.

7.3 Input distributions

Table 7.1 shows the means and standard deviations chosen to model the variable inputs in the Monte Carlo simulation. All these inputs were found to be normally distributed. The parameter values were obtained from plant data from July to October 2002. Figures 7.2 to 7.5 show the actual values of these variables over the time period. These variables

Table 7.1: Input distributions used in Monte Carlo modelling. All inputs are modelled with normal distributions.

Variable	Mean	Standard deviation	Units
Initial temperature	35	2,8	℃
Wood load	112	6,9	ton
Liquor load	188	6,4	m^3
CaO test value	1,074	0,039	weight % CaO

were chosen to be modelled due to the availability of data. It is important to realise that

these variables are by no means the only inputs that affect the final result of the cook.

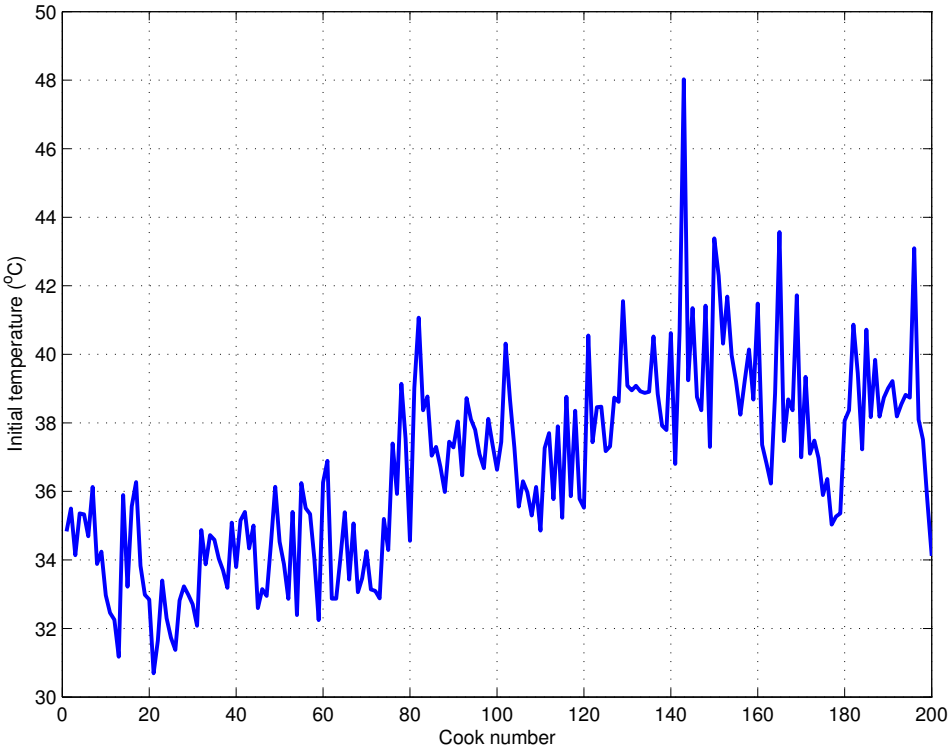

Figure 7.2: Initial temperature for cooks between July and October 2002

7.4 Methodology

Having broken up the model into its parts, each had to be implemented in a combination of MATLAB and Simulink. The distributions of the input variables were modelled as normal distributions based on data collected on the plant. The UP controller model is the same as the UP controller implemented on the real digester, while the S-factor controller was simulated based on documentation of the original implementation on the plant, as described in section 5.2.2.

Together, these models form a controlled system that can be subjected to known inputs and yield one output – the DP calculated at the end of the cook.

7.4.1 Monte Carlo model

Figure 7.6 shows the Simulink model that was created to model the digester and controllers. The shaded blocks represent the controller, the continuous variable generator (profile generator) and the digester itself. The profiles are simply output correctly by interpolating linearly between the turning points discussed in the previous sections. The digester and controller models are more involved and will be discussed below.

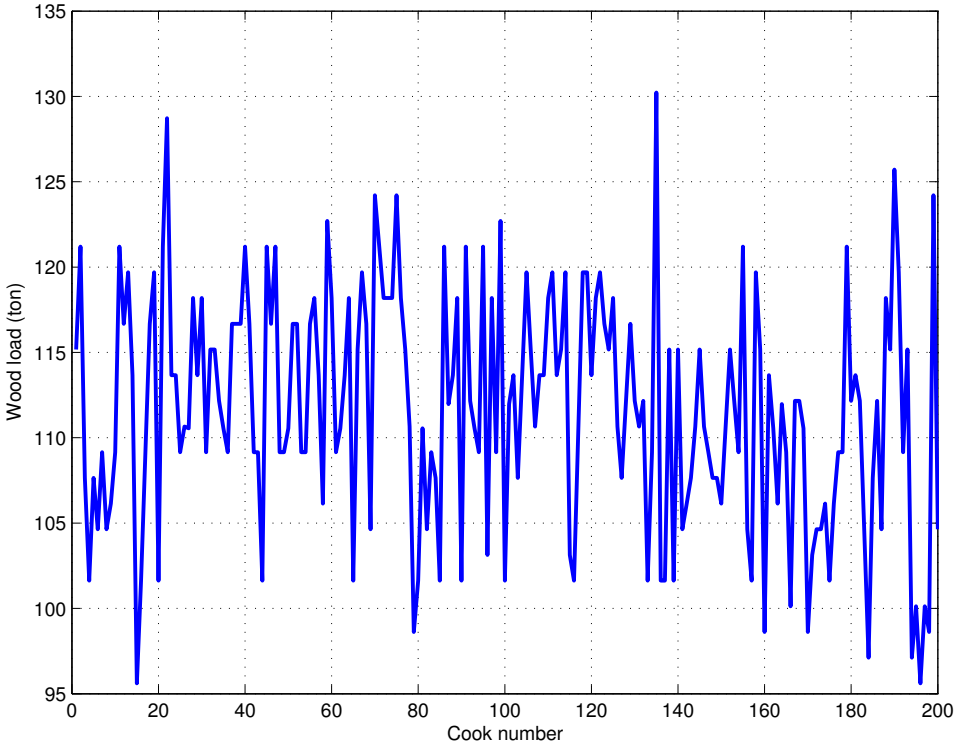

Figure 7.3: Wood load for cooks between July and October 2002

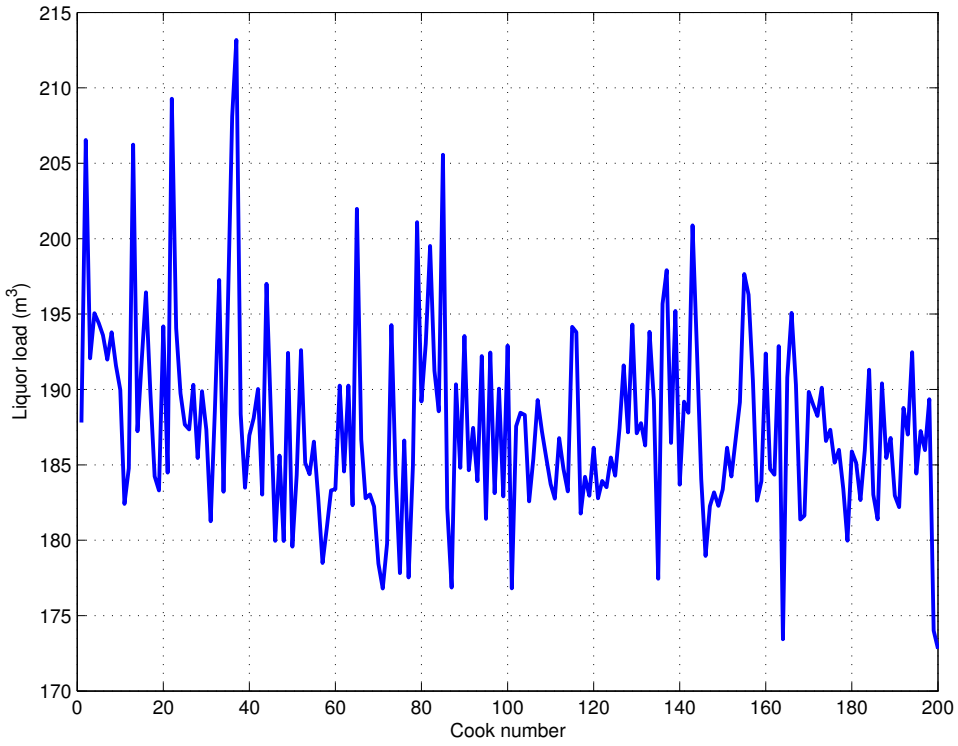

Figure 7.4: Liquor load for cooks between July and October 2002

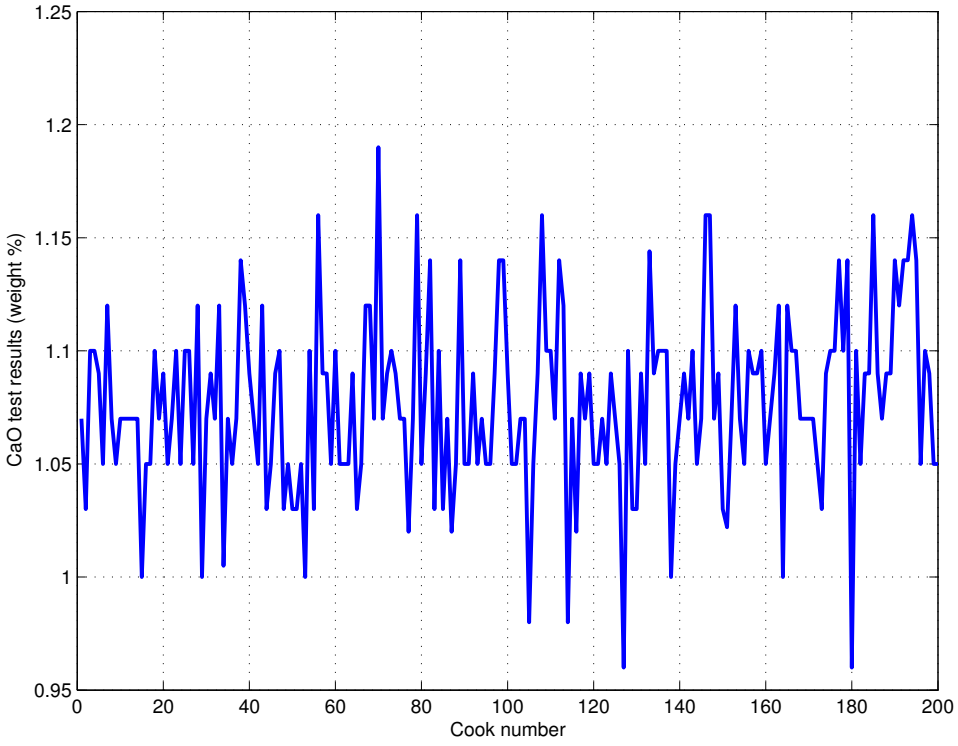

Figure 7.5: CaO test results for cooks between July and October 2002

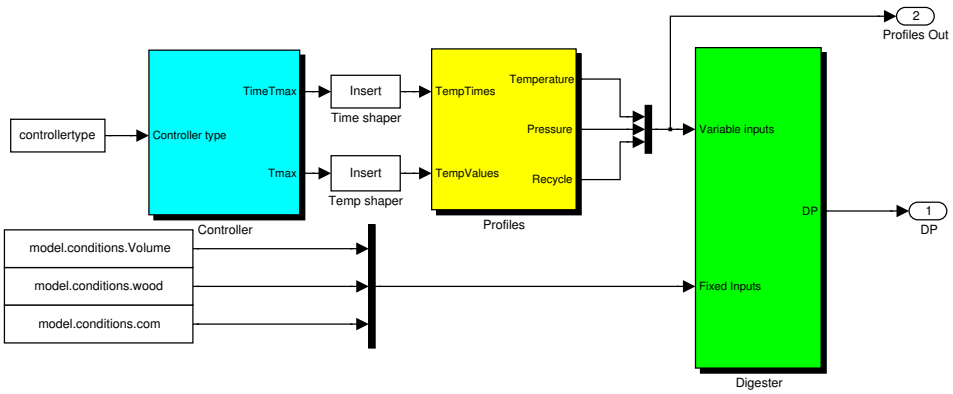

Figure 7.6: Simulink model for Monte Carlo simulation of the complete controller-digester system

7.4.2 Digester model

The digester model used in the simulation is based on the parameter values that Kilian (1999) arrived at during the model development. The controller uses this model to determine its control action as well. Therefore, the model used in the controller and in the digester are the same. This similarity will clearly cause the controller to perform well on the digester model.

The parameter values for the digester model were kept as they were reported by Kilian (1999) and the initial parameters used in the controller model were based on more recent cook data. The parameters used in the controller model differed from the digester model parameters sufficiently to ensure that the controller would not have an unrealistic advantage. The controller performance on the model without time to adjust its parameters was not perfect. Additionally, if the model of the process is good, it would correspond well to the conditions on the plant. A controller based on the same model would also have an advantage on this plant by design.

The exact model parameters used during simulation are shown in appendix A.

The Simulink implementation of the digester model is shown in figure 7.7

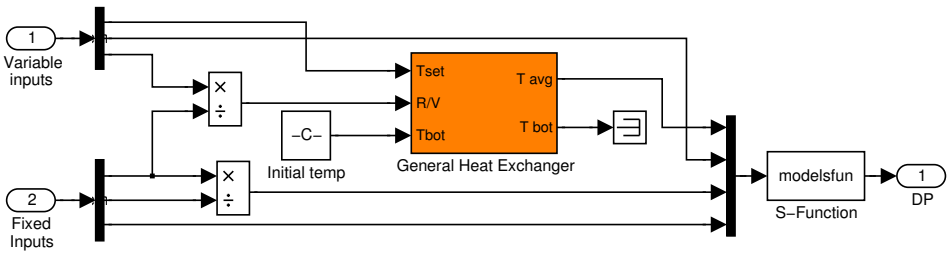

Figure 7.7: Simulink digester model for Monte Carlo simulation

7.4.3 Controller models

S-factor model

The S-factor algorithm described in paragraph 5.2.2 was modified slightly to enable efficient modelling of the controller. Instead of using a numeric summation for each time step, the rate equation (expressed by equation 5.2) was integrated numerically using a temperature profile generated as shown in figure 3.5, and the temperature that satisfied equation 5.8 found by numeric methods.

The calculation procedure can therefore be summed up as

- Calculate the target S-factor using equation 5.8 ($SF_{target} = A \times [SO_2^{free}]^2 + B \times [SO_2^{free}] + C \times (\%Base) + D$)
- Integrate the rate equation for the known temperature part (this is for time t_0 to time t_C). This is the part up to the final ramp to T_{top}. Set this integral equal to A_1

- Find T_{top} such that the remaining area (set equal to A_2) added to A_1 is equal to SF_{target}
- Use the value of $T_{m,top}$ in the temperature profile as shown in figure 3.5.

The parameter values used as a starting point for the S-factor controller are shown in table 7.2.

Parameter	Value
A	300
B	−3 200
C	4 000
D	7 000

Table 7.2: S-factor parameter values used in Monte Carlo modelling

To create a good baseline for worst-case performance of the S-factor controller, two different controllers were simulated. The first acts as a worst-case controller, and does not include the parameter update step described in paragraph 5.2.2. The second S-factor controller acts as described.

UP model

The UP model was initially loaded with parameters different from the model parameters used for the digester model. The parameters used as a starting point can be found in appendix A. The parameters were obtained by tuning the controller for optimal viscosity prediction on 20 cooks that took place during October 2002, before the Monte Carlo test was initiated.

7.5 Monte Carlo procedure

The result of a Monte Carlo simulation is inevitably a large number of data points. The determination of the response of a system in an instant in time is prescribed by looking at the distribution of many possible outcomes for that instant. The exact course the process will take given any one set of inputs is less important in such a study than the most probable route given the most probable inputs. It should be clear that the Monte Carlo simulation should have as many data points as possible to make a good estimate of the output distribution.

In order to simulate the training action of the UP controller and the adaptive action of the S-factor model, it was decided to model a run of 80 sequential cooks. This would give the controllers enough time to show the action of the adaption algorithms.

Here it is again important to bear in mind that the simulation involves many runs of 80 cooks for each controller. For each run, the controller will respond to randomly generated inputs conforming to the distributions described in the preceding sections, but will retain its parameters for that run. At the beginning of the next run, the parameters will be returned to their original state. The results for the simulation will be distributions obtained for the DP on each of the 80 cooks in sequence, showing the most likely action of the controller in light of the most likely inputs.

The simulation of so many cooks takes a significant amount of computer time. Even though one cook can be simulated in about 45 seconds on a Pentium III 800 (which is more than 600 times faster than real time), this simulation has to be repeated 3 times (one for each controller), and then 80 times for the sequential cooks. Simulating one run for all three controllers therefore takes 2 hours. Monte Carlo modelling dictates that the response of the system be measured for many different inputs conforming to the input model. It is clear that to generate any significant number of points quickly becomes a time consuming task.

In order to decrease the wall time that the simulation would take, it was executed on many computers at once, with the results combined after simulation. This is of course possible due to the way in which results are analysed – the order of simulations do not matter, since the inputs are randomly generated anyway. The only thing that is important in this study is that the 80 cooks be done in sequence, allowing the controllers to modify their parameters according to their algorithms, so that their adaptabiity can be evaluated.

The full source code of the program required to do the simulation once the models had been set up can be seen in the source code supplied on the CD.

The results of the Monte Carlo simulation are shown and discussed in chapter 9.

CHAPTER 8

Programming

The control strategy discussed so far has been implemented in a computer program running in the MATLAB environment. Before implementation of the program, a thorough analysis of the functionality required was made. The program was written using a modular strategy, ensuring the easy re-use of components in later developments. This chapter highlights the functional analysis and components created to implement the controller, as well as the Monte Carlo modeller.

8.1 Functional analysis

The program consists of parts with clearly defined roles. The functionality required from the program can be divided into four parts, namely

- Database interfacing
- User interfacing
- Modelling
- Optimisation

The two interfacing sections have been split as they are quite different – the database interface is on a computer-to-computer basis, while user interface is between the user and the computer.

The modelling of the reactions inside the reactor is done by a group of Simulink models similar to those created by Kilian (1999). These models can be used to simulate a complete cook and are used to predict a setpoint during control or the DP during optimisation.

It should be noted that there are two optimisation stages in the normal operation of the controller. In the short term (per cook), there is an optimisation used to determine the correct value of $T_{m,top}$ for a target DP value. In the N cooks time frame, the model parameters are changed to match historical values. The optimisation of the model parameters is done by minimising the error (given as a COV) of the model predictions of cooks for which DP results are available compared to the true DP as obtained from laboratory results.

8.2 Data flow

To facilitate control, data have to be transfered between the different components. Figure 8.1 shows the major dataflows between systems.

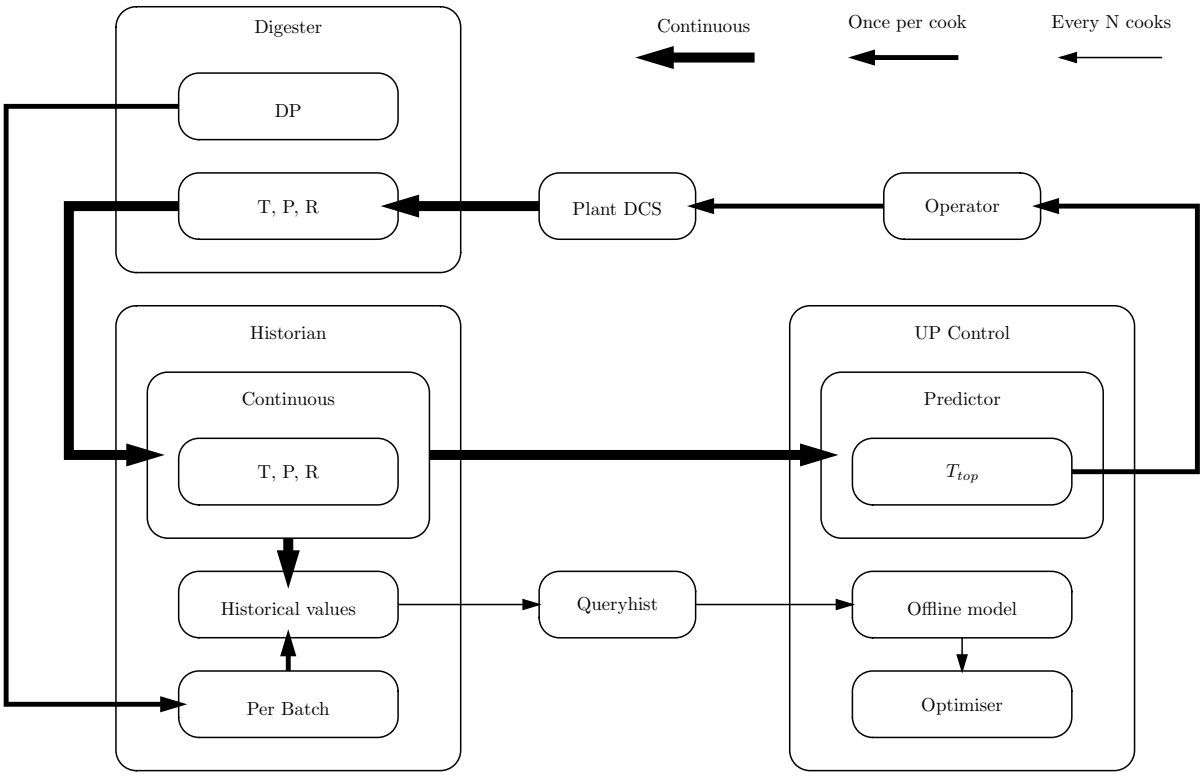

Figure 8.1: Data flow in the UP control program

Two main data cycles can be identified in figure 8.1. One cycle is on a continuous time scale, reading continuous plant data from the historian system and using these data as inputs for the running model. The second cycle used by the offline optimisation routines, reading stored plant data from the historian in bulk and using these data to optimise the model parameters.

It should also be noted that the connection shown between the control program and the online system controlling the temperature on the digester is not electronic, but involves

displaying the desired value on the computer screen and allowing plant personnel to enter the maximum temperature.

8.2.1 Continuous time frame

The data read continuously are used directly in the process model. They are not stored during the cook process, as this was found to be too slow to allow real time processing.

During the control simulation, feedback is given to the personnel using the software by updating graphics on the user interface showing the current temperatures, side circulation flow rate and pressure read from the plant, as well as the values of the calculated pH and estimated DP.

The different phases of the control problem require separate action. The initial phase, until the one hour test becomes available, simply stores data during this phase. Once the data becomes available, it is used to deduce the starting conditions of the digester.

8.2.2 Per cook time frame

Before and after each cook, parameters must be loaded into the controller variables, the graphical display must be updated to show that no cook is in progress, and data pertaining to the cook that has just been run must be stored for later analysis. Also, after each cook, a decision has to be made on whether to optimise parameters or not. At the moment, the program uses a 10 cook interval for parameter tuning.

8.2.3 N cook time frame

After N cooks have passed (at the moment $N = 10$), the parameters have to be optimised to ensure the best fit between the model predictions and the real results of the previous N cooks. This is done using MATLAB's built in optimisation routines which are based on the Simplex method.

8.3 Functional dependence

Figure 8.2 shows the functional dependence diagram for the program. This file is also available on the CD-ROM accompanying the dissertation. This diagram proved invaluable in the debugging of the program and in building new functions. It should also be of use during porting of the program to other platforms. The Graphviz program produced by the AT&T computer laboratories was used to generate the diagram using data obtained by a separate MATLAB program written by the author of this dissertation that scans the a MATLAB program directory for functional dependencies.

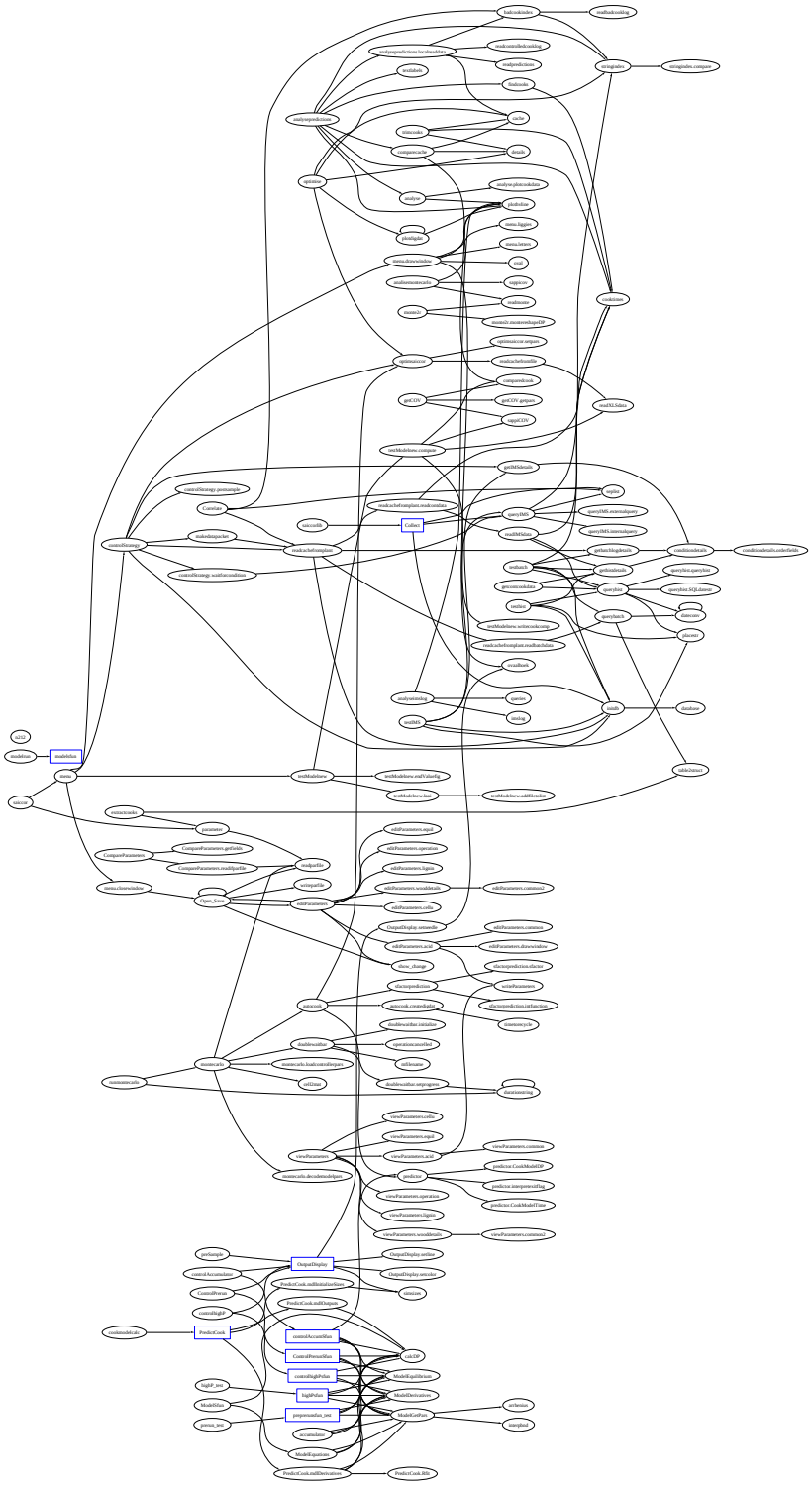

Figure 8.2: Functional dependance of modules in the program

8.4 Matlab programs

The MATLAB programs used to implement the controller and the Monte Carlo simulation are available on the CD that accompanies this dissertation due to space constraints.

When perusing the programs, it should be noted that uniform style and documentation was used. This is to ensure that the program is legible and easily portable to other platforms if the need should arise.

8.5 Simulink models

Several Simulink models were developed as part of the programming effort. The description here is included as the precise functioning of Simulink models are often hard to fathom without some comments.

8.5.1 Database read block

The database read block shown in figure 8.3 allows access of offline or online data in a manner that is transparent to the rest of the Simulink models. This means that the same

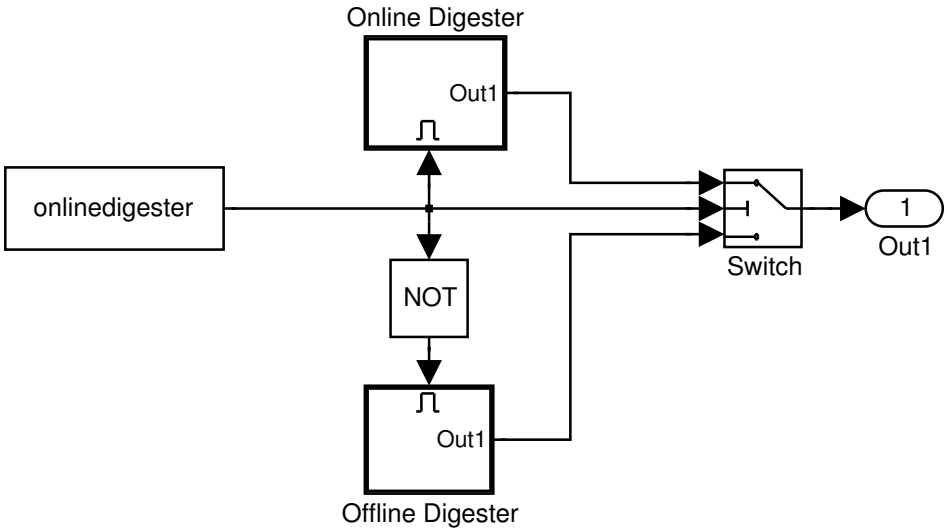

Figure 8.3: Database read block

models can be used to simulate both online and offline conditions. This is achieved by using two blocks which are enabled and disabled using a flag (`onlinedigester`) which is true when digester is online. This flag not only enables the correct block, but switches the system output to be connected to the correct block as well.

8.5.2 Heat exchanger block

The heat exchanger block shown in figure 8.4 is used to model the temperature of the digester by assuming the digester can be modelled by several well mixed stages. The

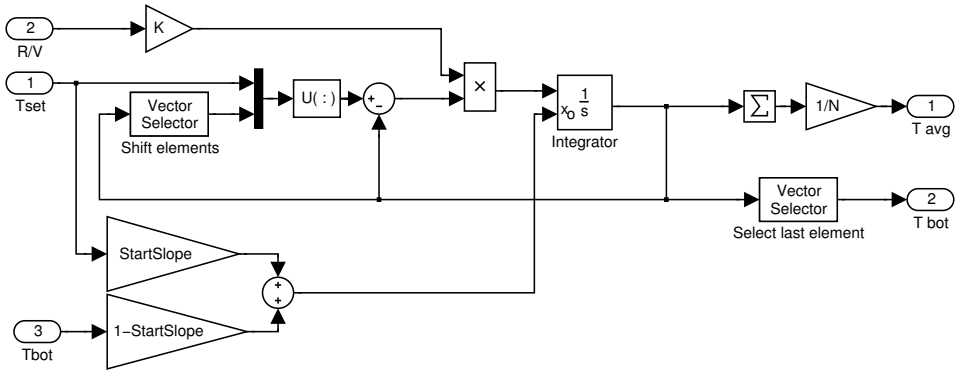

Figure 8.4: Heat exchanger model

model has been constructed so that the number of subdivisions can be entered by the user during the setup of the model. The integrator then models the temperature of all the subdivisions. The model requires the current ratio of the recycle to the initial volume in the digester (`R/V`), the current temperature setpoint (`Tset`) and the initial bottom temperature (`Tbot` on the left). It returns the current average and bottom temperatures predicted for the digester (`Tavg` and `T bot` on the right).

8.5.3 Phase models

During the various phases of a cook, different models are called, each terminating on preset conditions. They are set up differently to accommodate the differences in operating conditions and the data available to the program at that stage of the cook.

Figure 8.5 shows the model which is run to collect data until the sample results become available. It reads from the database, recording all the variables that are read every minute (in the file `presamplesigdat`). It also checks whether the test result is available by comparing the current database entry to the default value for the test result. Once the data becomes available, the result will be higher than the default and the model will terminate.

After the sample data becomes available and the presample model has completed running, the prerun model shown in figure 8.6 is called to simulate the cook up to the point where the data became available.

This model reads stored data (`digdat`) from the workspace and simulates faster than real time to catch the simulation up past the time where the sample was taken, so that the simulation time corresponds to real time.

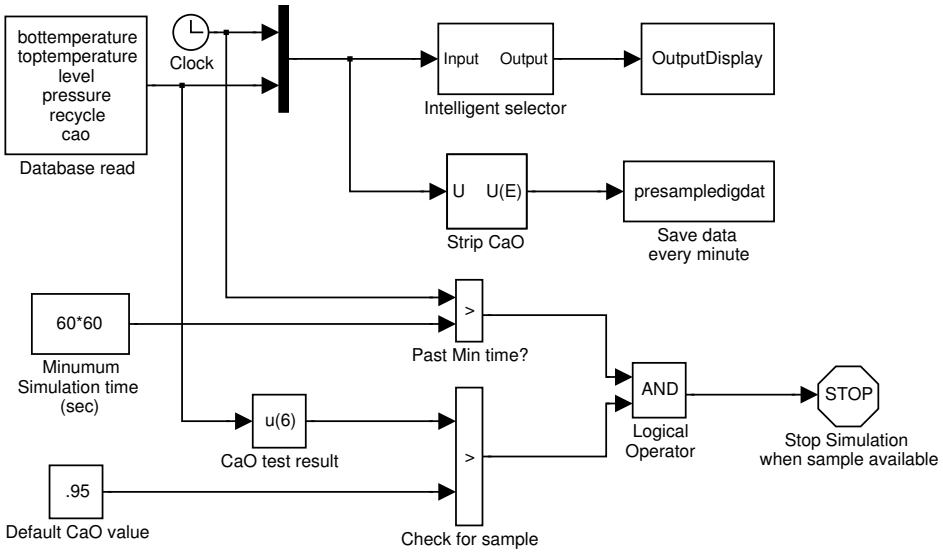

Figure 8.5: Presample model

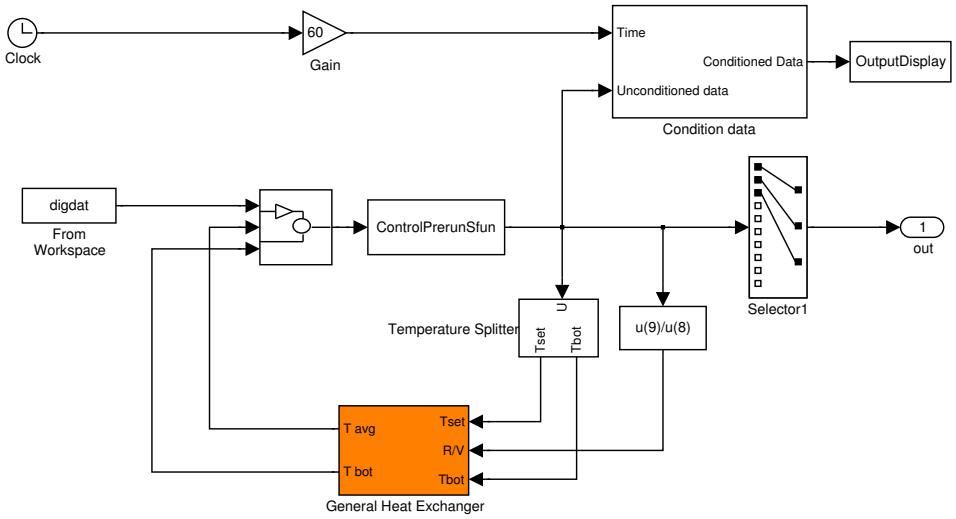

Figure 8.6: Prerun model

Now that the simulation is up to date, the Accumulator model shown in figure 8.7 is called to run real-time simulation and call the prediction routine when the temperature reaches the final ramp stage.

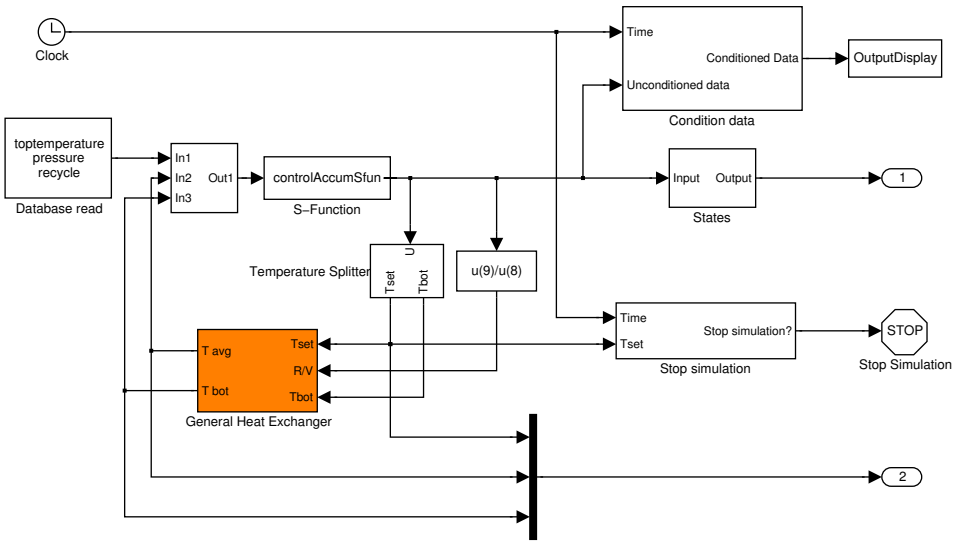

Figure 8.7: Accumulator model

The accumulator model runs until the temperature reaches the target and the pressure is in the final high pressure zone. At this point the High pressure phase model shown in figure 8.8 is called to simulate the final stages of the cook.

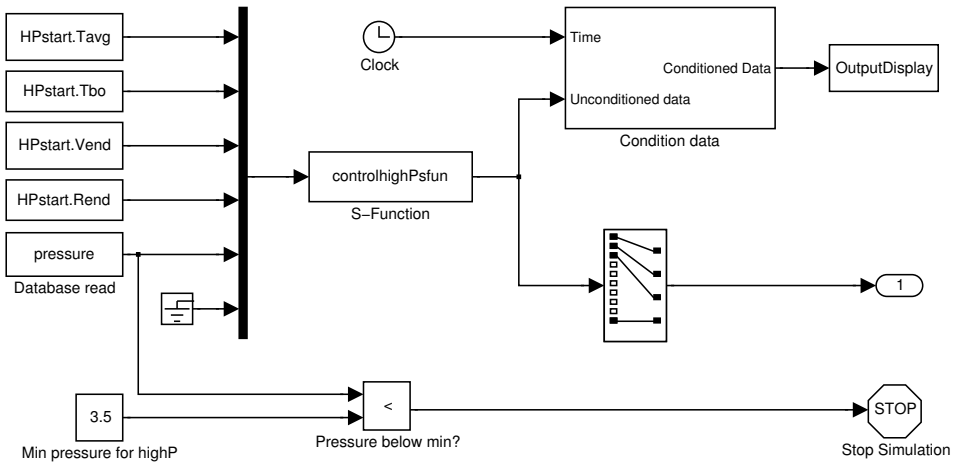

Figure 8.8: High pressure phase model

All of these models use the same output function, `outputdisplay` to update the graphics on the user interface and keep the user informed of the actions of the program and the controller.

8.6 CD-ROM

The typeset version of the source code as well as the MATLAB executable source code for the program is available on the CD-ROM which accompanies this dissertation. The programming language used is MATLAB, but some functions (like SQL calls to the database and compression of log files) were performed using external programs. The SQL query program was provided by Saiccor and the compression tool used was 7-zip, a free program distributed under the GPL.

CHAPTER 9

Results

The results of both the Monte Carlo modelling and the *in-situ* controller trials are discussed in this chapter. The basis for the performance coefficient is calculated and performance of the current controller as well as the *in-situ* UP controller are calculated.

9.1 Monte Carlo

9.1.1 Statistical validity

Table 9.1 shows the details of the simulation results gathered. The total computer time spent on the simulation was more than 25 days. This was split over 5 computers, resulting in more than 5 days being spent on the simulation, as not all the computers were equally fast.

Using the Kolmogorov-Smirnov test (as described in section 2.10.3), the outputs can be shown to be normally distributed within reasonable limits for areas where the controller tuning remains constant. Figure 9.1 shows the KS distance and the critical distance for $\alpha = 5\%$ for the individual time steps in the Monte Carlo simulation results. It can be seen from this graph that the KS distance is below the critical distance in all cases. Space does

Table 9.1: Details of Monte Carlo simulation

Parameter	Value
Cooks per run	80
Runs	200
Input variables	4

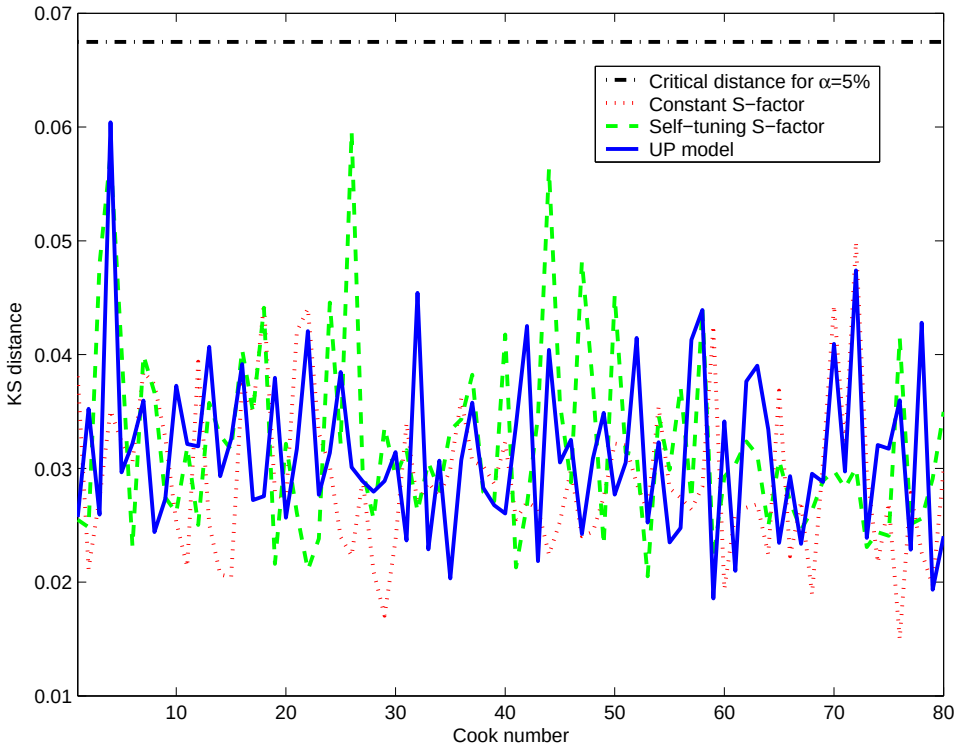

Figure 9.1: Kolmogorof-Smirnov test results for Monte Carlo simulation. The critical distance for $\alpha = 5\%$ is shown.

not permit showing the graphical representation of the Kolmogorov-Smirnov test for all the cooks in the Monte Carlo simulation, as this would involve 80 graphs per controller.

Figure 9.2 shows the cumulative distribution function (CDF) for DP resulting from cooks between January and February 2003, as well as the fitted true normal CDF. The Kolmogorov-Smirnov test result (KS distance) is the largest distance between these two curves. The critical distance for $\alpha = 5\%$ is 0,134, while the KS distance for this distribution is 0,088, allowing us to assume that the distribution is indeed normal.

The good normality results make it possible to assume normally distributed results will be the norm. The standard deviation and means of results obtained will therefore be justifiable, even for a small number of data points.

9.1.2 Output distribution

Figure 9.3 shows the distributions obtained for the different controllers. It is clear from the figure that the UP controller gives an overall output variance which is less than that of the S-factor controllers. It should however be noted that the distributions shown here are for the controlled variable over all 80 of the cooks in a run and are not perfectly normal. This is because of the control action that changes the variance and mean with time. Note that the UP controller 'leans' more toward the target than the self-tuning S-factor controller and that the S-factor controller which does not have its parameters adapted is

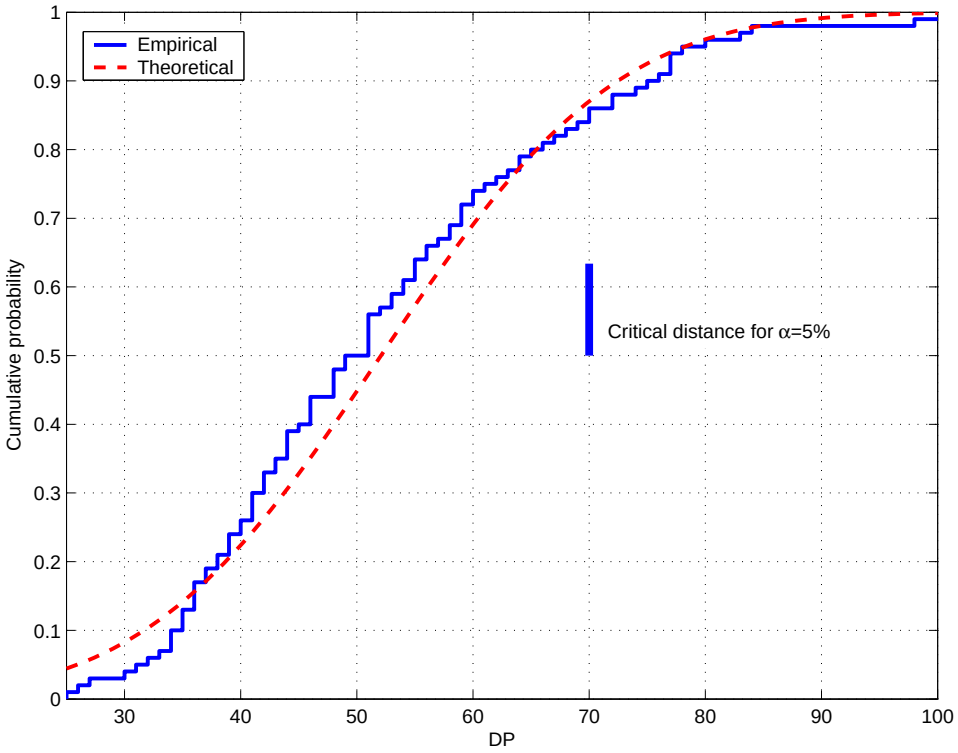

Figure 9.2: Kolmogorov-Smirnov test graph for DP of cooks between January and February 2003. The critical distance for $\alpha = 5\%$ is shown for comparison.

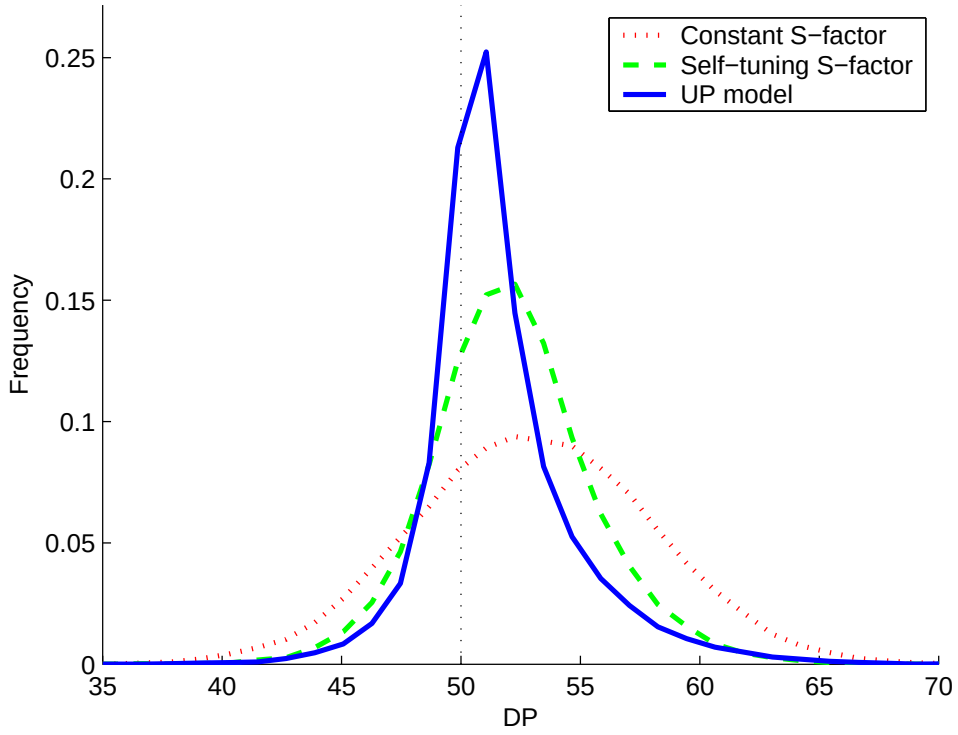

Figure 9.3: Overall distributions obtained with different controllers via Monte Carlo simulation. The target DP is 50.

perfectly symmetric, as is to be expected. The peak in the UP controller's distribution is due to the size of the bins used to draw the distribution. Due to the number of datapoints, the number of bins could not be made less without losing smoothness elsewhere in the graph.

In order to see the performance of the online tuning of the UP controller and the self-tuning S-factor controller, it is necessary to visualise the results over time. Figure 9.4 shows the results of the simulation versus the cook number. In this figure the reduction

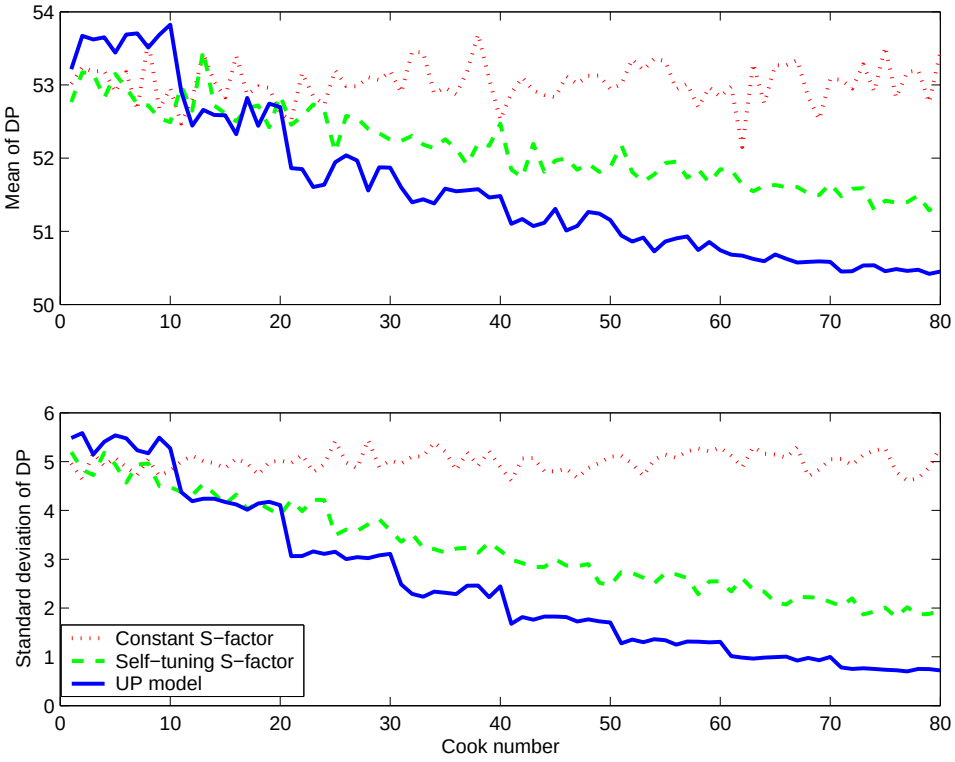

Figure 9.4: Monte Carlo results over time

of both variance and error over time brought about by the adaptive algorithms can be seen. The constant parameter S-factor controller does not exhibit any time-dependent behaviour.

9.2 Performance criteria

Based on the Monte Carlo results, it can be seen that the simulated UP controller shows the smallest output variance. The standard deviation obtained over all the cooks was calculated as 3,07. It was decided to use the standard deviation of the viscosity error as the performance measure for the controller, combined with the mean of the error (which should be zero), this gives a good picture of the controller performance. Therefore, control performance is expressed by using the measured variance divided by 3,07 as well as the mean of the error.

9.3 In situ control results

9.3.1 Results

The UP controller was used to control 13 cooks during the period from May 2003 to June 2003. Figure 9.5 shows the performance of the S-factor controller during the same period. The horizontal dashed line shows an average deviation from target slightly above 10. Note that the DP cycles dramatically between high and low extremes during this time period. This is typical of the overall operation of the controller.

Several reasons for this cyclic behaviour can be suggested. The most likely explanation is aggressive modification of the controller parameters by plant personnel, without waiting for the effects of these modifications.

Figure 9.6 shows the performance of the UP controller during the same time period. The vertical line shows the point at which new model parameters were obtained using the automatic tuning facility. When comparing the two controllers, it should be noted that the S-factor controller parameters are changed for almost every cook. This makes it difficult to identify contiguous regions where the same parameters are used, as was done in the figure showing UP controller performance.

The figures show clear evidence of the superiority of the UP controller. After parameter tuning, the deviation from target was significantly lowered, and the variance is consistently lower than that of the S-factor controller during the same time period.

It should be noted that the variances measured on the plant are consistently higher than those obtained using Monte Carlo simulation. This is because the Monte Carlo model only introduces variability in the variables that are measurable on the plant. Many more unmeasured variables play a part in determining the final viscosity, and will add cause the final output to have larger variance. In addition, there is variability in the plant model which was not taken into account. Varying the values of the plant model parameters will add an addition measure of reality. Unfortunately, there was not enough data to develop an estimate of the plant model parameter distributions.

9.3.2 Variance reduction

The variance of S-factor controller during the test was measured as 21, 7 times the value obtained by Monte Carlo analysis. The UP controller variance was at 18 before parameter tuning and at 12 after parameter tuning, 6 and 4 times the theoretical values respectively. The Monte Carlo results suggest that this figure can be expected to drop further when the parameters are tuned again. Even if the variance does not improve, the UP controller shows a 43% lower variance.

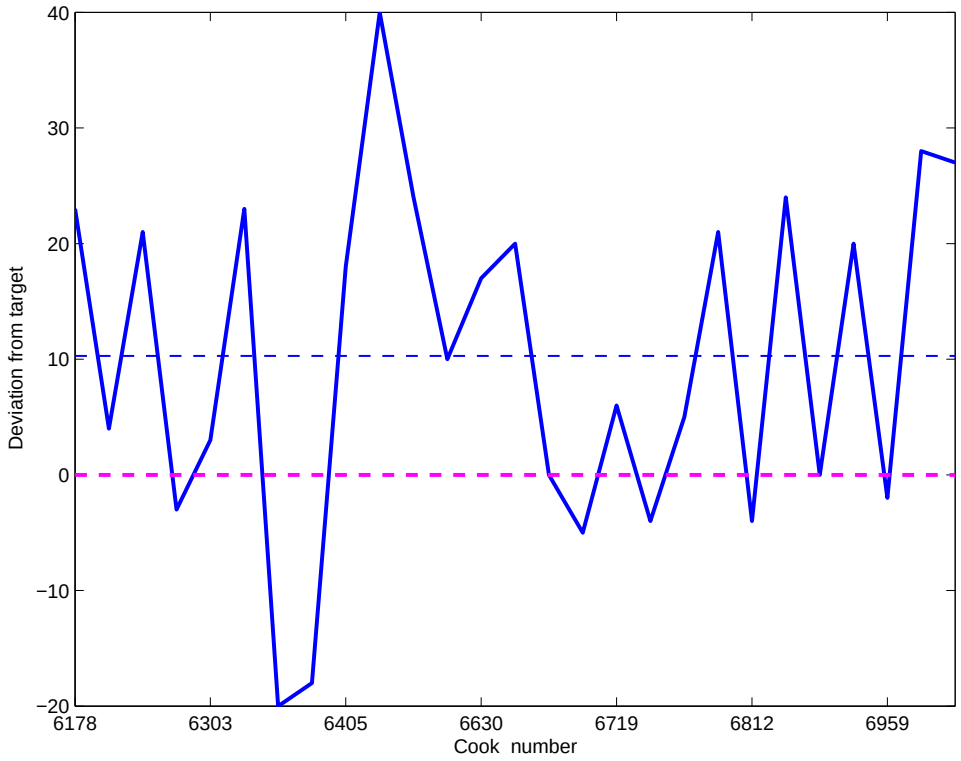

Figure 9.5: Deviation from target for S-factor controller May to June 2003

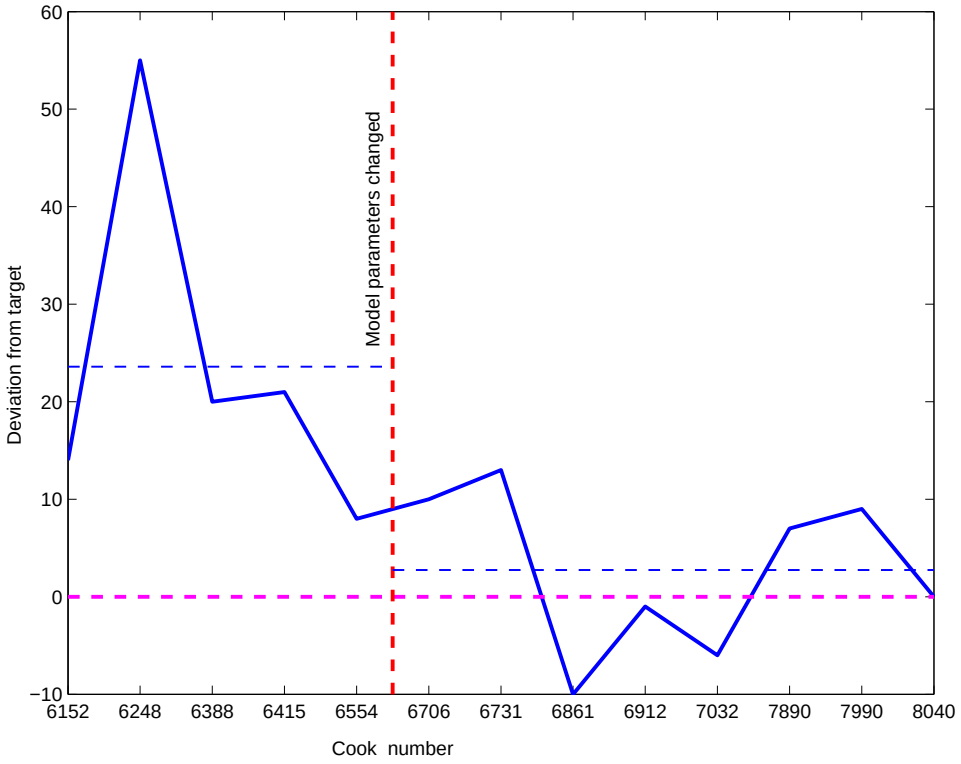

Figure 9.6: Deviation from target for UP controller May to June 2003

9.3.3 Error reduction

The UP controller showed an average error of only 1 unit after parameter tuning, and Monte Carlo modelling suggests that this value may decrease if the plant conditions stay constant. The S-Factor controller showed an average error of 10 units. The high average error can be explained by the fact that personnel are loathe to obtain low viscosities. Given that the S-factor controller exhibits a high variance, average viscosities are consistently high to avoid low viscosity results.

CHAPTER 10

Conclusion and recommendations

This chapter summarises the findings of this study and makes recommendations for further research and investigation.

10.1 Monte Carlo modelling

The results of the Monte Carlo experiment show that the UP controller performs better than the current controller on the plant. The study also shows evidence of variability in unmeasured variables when compared to the real plant data, as the real plant data shows higher output variance than the simulation. In addition to the effects of unmeasured process variables and variable process parameters on the variance, the mismatch in variability between simulation and reality could be that current parameter tuning technique used to adjust the S-factor controller parameters to maintain control on the plant.

10.2 In-situ controller

The UP controller program has been shown to correctly predict temperatures in an online plant environment. The controller showed a significantly (42%) lower variance than the current (S-factor) controller during the same period, and also showed a 64% reduction in average error. The effect of parameter tuning was also observed to be significant and correlated well with the Monte Carlo results.

10.3 Controller structure

The UP controller structure is based on a simple concept – that of feedforward control with adaptable parameters. Many different concepts were evaluated during the design.

It has been mentioned (chapter 1) that state estimation techniques are not directly applicable to this specific problem.

Other control structures which might seem attractive include Neural Networks or more automated model based techniques such as MRAC. These techniques all have the disadvantage of not being based on a rigorous model, but rather being reliant on historic data to predict the behaviour of the plant. Due to the fact that the digester does not exhibit continuous change and the extremely low sampling rate of the controlled variable, these techniques can only approach a model based on knowledge of the internal reactions and adjusted periodically.

10.4 Recommendations

A number of issues were identified during the course of this investigation, which took place over a total of five years.

- Further study into sources of variability has to be done, as it is clear that the model used by the UP controller does not account for all the variability observed on the plant. If these sources of variability can be identified, they might provide valuable clues as to further ways of reducing the output variance.

- The possibility of adding additional measurements is also an interesting field for further study. One additional measurement such as near-infra-red spectrum analysis or moisture content measurements of wood entering the digester could improve control by allowing the model to use correct initial values for the model rate equations.

- If the controller can obtain optimised parameters for different species of wood, these parameters could be stored for recall when switching wood species.

- Control can be improved considerably by removing the constraint that the cook time needs to be constant. The control algorithm can be easily adapted to supply an optimal time for a constant temperature profile instead of an optimal temperature for a constant time cook.

- In order for variable time cooks to be possible, scheduling on the plant has to be reworked. The current constant time constraint is due to the difficulty of manually scheduling the digesters taking into account shared equipment and utilities. If the scheduling could be automated, the constant time constraint could be relaxed.

- The model of the reactions used in this study are rigorous enough that they may be incorporated into training simulations.

- The Monte Carlo modelling structure can be used to evaluate any control structure and will aid in the evaluation of the impact of process changes or any of the opportunities mentioned above.

APPENDIX A

Parameter values

These values are the original values for the model parameters as published by Kilian (1999), together with the modified values used as a starting point in the UP controller during Monte Carlo testing and the parameters obtained through parameter optimisation using gathered plant data.

Table A.1: Lignin reaction kinetics

	Literature (Kilian, 1999)		Monte Carlo		Plant	
Parameter	$[L] > 12$	$[L] < 12$	$[L] > 12$	$[L] < 12$	$[L] > 12$	$[L] < 12$
K_{L0}	$1{,}415 \times 10^{12}$	$4{,}278 \times 10^{11}$	$1{,}414\,8 \times 10^{12}$	$4{,}278\,2 \times 10^{11}$		
E_L	12 300	12 300	$1{,}233\,4 \times 10^{4}$	$1{,}232\,6 \times 10^{4}$	12 300	12 300
a	0,646	1,621	1,028 5	2,536 6	0,646	1,621
α	0,819	0,765	0,718 6	0,425 1	0,819	0,765
β	0,705	0,778	0,428 3	0,552 9	0,705	0,778

Table A.2: Hemicellulose reaction kinetics

Parameter	Literature (Kilian, 1999)	Monte Carlo	Plant
K^0_{HC}	$1{,}236 \times 10^{11}$	$1{,}238 \times 10^{11}$	$1{,}226 \times 10^{11}$
E_{HC}	14 200	14 370	14 300
d	2,542	2,322	2,741
γ	0,707	0,710	0,723

Table A.3: Cellulose reaction kinetics

Parameter	Literature (Kilian, 1999)	Monte Carlo	Plant
K^0_C	$7{,}68 \times 10^{12}$	$1{,}543 \times 10^{13}$	$4{,}32 \times 10^{12}$
E_C	17 100	$1{,}724 \times 10^{4}$	$2{,}34 \times 10^{4}$
δ	1	1,643	1,434

Table A.4: Interpolation tables for B and C

		Literature (Kilian, 1999)		Monte Carlo		Plant	
Parameter	Temp (°C)	B	C	B	C	B	C
$K^0_{SO_2}$	80	−5,077	1 045	−5,077 0	1 045	−5,077	1 045
	120	−6,16	−6,916 0	1 700	1 700	−6,16	1 700
	150	−7,71	2 133	−7,971 0	2 113	−7,71	2 133
K_P	80	−10,212	2 392	−10,241	2 392	−10,212	2 392
	120	−10,125	2 669	−10,130	2 665	−10,125	2 665
	150	−11,348	2 960	−11,230	2 960	−11,348	2 960
K_{H_2O}	20-150	5,648	−2 198	5,648	−2 198	5,648	−2 198

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